EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	6078980	"alzheimer's" "beta-secretase activity" inhibition mammal prevent? control? reduc?	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	OR	ON	2007/06/20 17:15
L2	35	"alzheimer's" "beta-secretase activity" inhibition mammal prevent? control? reduc?	US-PGPUB; USPAT; USOCR; FPRS; EPO; JPO; DERWENT	AND	ON	2007/06/20 17:15

```
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 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  MAR 15  WPIDS/WPIX enhanced with new FRAGHITSTR display format
 NEWS  3  MAR 16  CASREACT coverage extended
 NEWS  4  MAR 20  MARPAT now updated daily
 NEWS  5  MAR 22  LWPI reloaded
 NEWS  6  MAR 30  RDISCLOSURE reloaded with enhancements
 NEWS  7  APR 02  JICST-EPLUS removed from database clusters and STN
 NEWS  8  APR 30  GENBANK reloaded and enhanced with Genome Project ID field
 NEWS  9  APR 30  CHEMCATS enhanced with 1.2 million new records
 NEWS 10  APR 30  CA/CAplus enhanced with 1870-1889 U.S. patent records
 NEWS 11  APR 30  INPADOC replaced by INPADOCDB on STN
 NEWS 12  MAY 01  New CAS web site launched
 NEWS 13  MAY 08  CA/CAplus Indian patent publication number format defined
 NEWS 14  MAY 14  RDISCLOSURE on STN Easy enhanced with new search and display
                  fields
 NEWS 15  MAY 21  BIOSIS reloaded and enhanced with archival data
 NEWS 16  MAY 21  TOXCENTER enhanced with BIOSIS reload
 NEWS 17  MAY 21  CA/CAplus enhanced with additional kind codes for German
                  patents
 NEWS 18  MAY 22  CA/CAplus enhanced with IPC reclassification in Japanese
                  patents
 NEWS 19  JUN 18  CA/CAplus to be enhanced with pre-1967 CAS Registry Numbers

 NEWS EXPRESS  NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT
               MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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FILE 'HOME' ENTERED AT 17:42:12 ON 20 JUN 2007

=> file registry
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                      ENTRY    SESSION
FULL ESTIMATED COST                                    0.21       0.21
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STRUCTURE FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1
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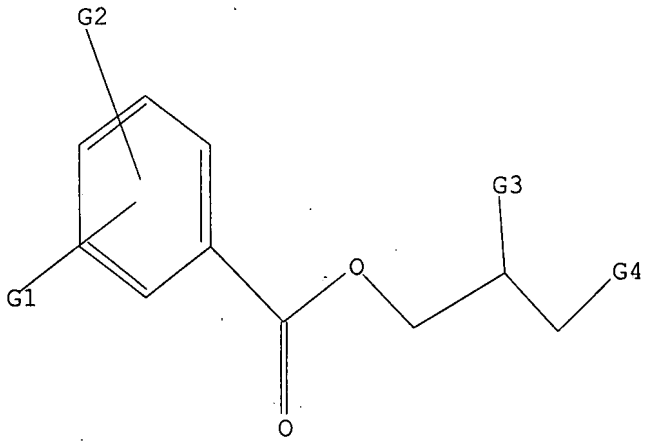
=>
Uploading C:\Documents and Settings\jcho2\My Documents\10562470-1.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 C,O

G2 N,Ph

G3 O,N

G4 Ph,O

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 17:43:24 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 45746 TO ITERATE

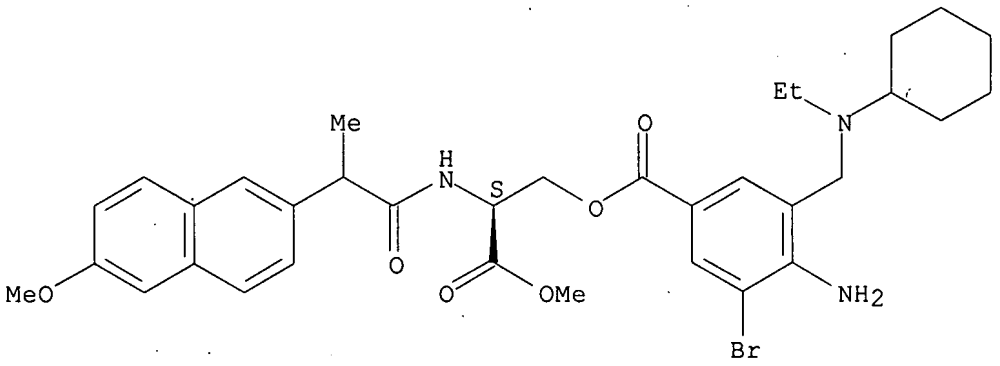
100.0% PROCESSED 45746 ITERATIONS 88 ANSWERS
SEARCH TIME: 00.00.01

L2 88 SEA SSS FUL L1

=> d scan

L2 88 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN L-Serine, N-[2-(6-methoxy-2-naphthalenyl)-1-oxopropyl]-, methyl ester, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate (ester) (9CI)
MF C34 H42 Br N3 O6

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):file caplus
'FILE CAPLUS' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END".
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	172.55	172.76

FILE 'CAPLUS' ENTERED AT 17:43:46 ON 20 JUN 2007
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FILE COVERS 1907 - 20 Jun 2007 VOL 146 ISS 26
FILE LAST UPDATED: 19 Jun 2007 (20070619/ED)

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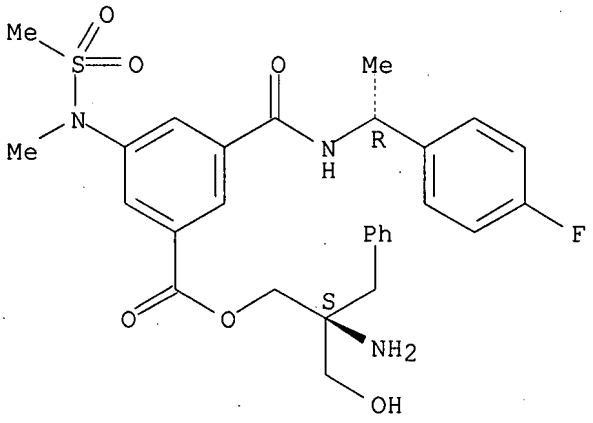
http://www.cas.org/infopolicy.html

=> s l2
L3 30 L2

=> d l3 1-30 bib abs hitstr

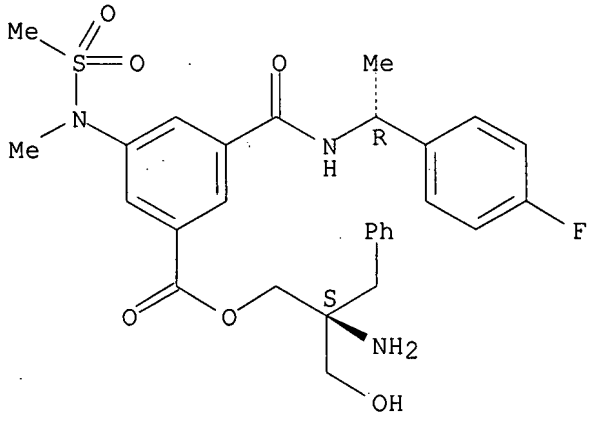
L3 ANSWER 1 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1191598 CAPLUS
DN 146:116781
TI Discovery of Oxadiazoyl Tertiary Carbinamine Inhibitors of β-Secretase (BACE-1)
AU Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Munshi, Sanjeev; McGaughey, Georgia B.; Lindsley, Stacey R.; Young, Mary Beth; Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis; Pietrak, Beth; Crouthamel, Ming-Chih; Tugusheva, Katherine; Huang, Qian; Xu, Min; Simon, Adam J.; Kuo, Lawrence; Hazuda, Daria J.; Graham, Samuel; Vacca, Joseph P.
CS Departments of Medicinal Chemistry, Structural Biology, Molecular Systems and Alzheimer's Research, Merck Research Laboratories, West Point, PA, 19486, USA
SO Journal of Medicinal Chemistry (2006), 49(25), 7270-7273
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 146:116781
AB We describe the discovery and optimization of tertiary carbinamine derived inhibitors of the enzyme β-secretase (BACE-1). These novel non-transition-state-derived ligands incorporate a single primary amine to interact with the catalytic aspartates of the target enzyme. Optimization of this series provided inhibitors with intrinsic and functional potency comparable to evolved transition state isostere derived inhibitors of BACE-1.
IT 918344-77-1 918344-77-1D, complexes with β-secretase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(discovery of oxadiazoyl tertiary carbinamine inhibitors of β-secretase)
RN 918344-77-1 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 918344-77-1 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.

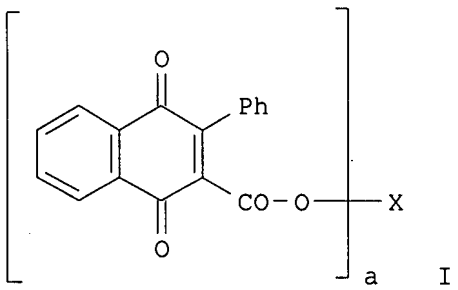


RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:125835 CAPLUS
DN 144:202124
TI Phenylnaphthoquinones, and their electrophotographic photoconductors showing good durability and solvent resistance
IN Ichiguchi, Tetsuya
PA Kyocera Mita Industrial Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 47 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

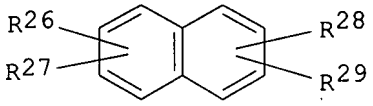
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2006036677	A	20060209	JP 2004-217855	20040726
PRAI	JP 2004-217855		20040726		

OS MARPAT 144:202124
GI



I

II



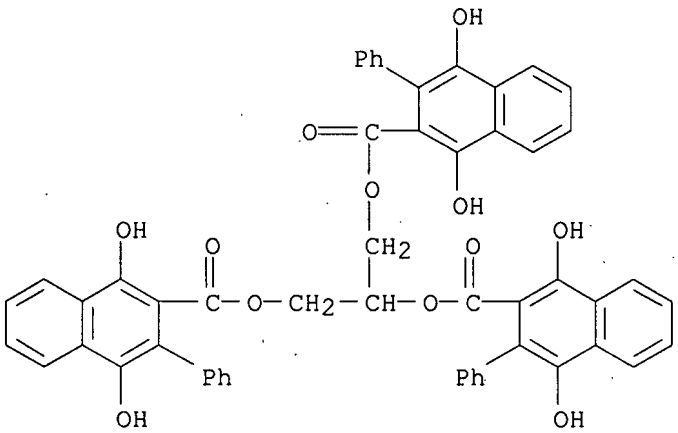
III

AB The naphthoquiones are I (X = trivalent group chosen from C6H3R1R2R3, R4CHR5R6, etc. when a = 3, tetravalent group chosen from tetravalent benzene II, tetravalent naphthalene III when a = 4; R1-R3, R22-R29 = single bond, C1-8 alkylene, C2-8 alkylidene, etc.; R4-R6 = single bond, C1-4 alkylene). The electrophotog. photoconductors contain charge generating agents, I as electron transporting agents, and binder resins. Thus, I (X = 1,3,5-benzenetrimethylene, a = 3) was manufactured and used for an electrophotog. photoconductor.

IT 875078-03-8P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(phenylnaphthoquinones as electron transporting materials for electrophotog. photoconductors showing good durability and solvent resistance)

RN 875078-03-8 CAPLUS

CN 2-Naphthalenecarboxylic acid, 1,4-dihydroxy-3-phenyl-, 1,2,3-propanetriyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 3 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 2005:55021 CAPLUS

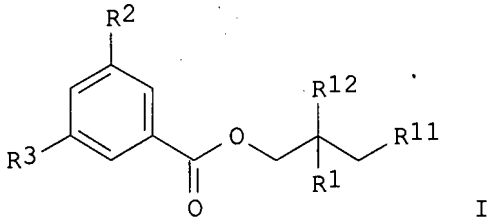
DN 142:134323

TI Preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease

IN Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005004803	A2	20050120	WO 2004-US20525	20040625
	WO 2005004803	A3	20050421		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2004255191	A1	20050120	AU 2004-255191	20040625
	CA 2530006	A1	20050120	CA 2004-2530006	20040625
	EP 1643986	A2	20060412	EP 2004-756168	20040625
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	CN 1909897	A	20070207	CN 2004-80018651	20040625
	US 2006149092	A1	20060706	US 2005-562470	20051222
PRAI	US 2003-484150P	P	20030701		
	WO 2004-US20525	W	20040625		

OS MARPAT 142:134323
GI



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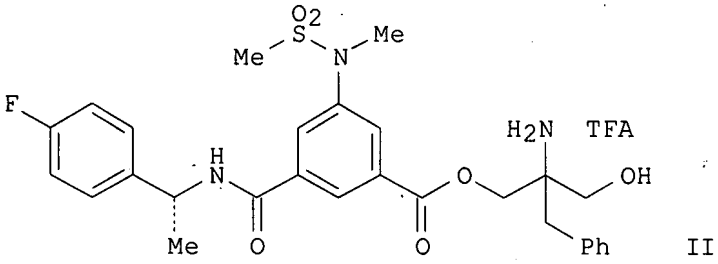


II

AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl, alkenyl, alkynyl, Ph, PhCH2; R7 = H, alkyl, alkenyl, alkynyl; R3 = (substituted) PhCHR5NHCO, R9R10NHCO, etc.; R9R10 = atoms to form (substituted) pyrrolidinyl, piperidinyl; R11 = OH, alkoxy, phenylalkoxy, PhO, Ph; R12 = NR9R10, OH], were prepared as β-secretase inhibitors for

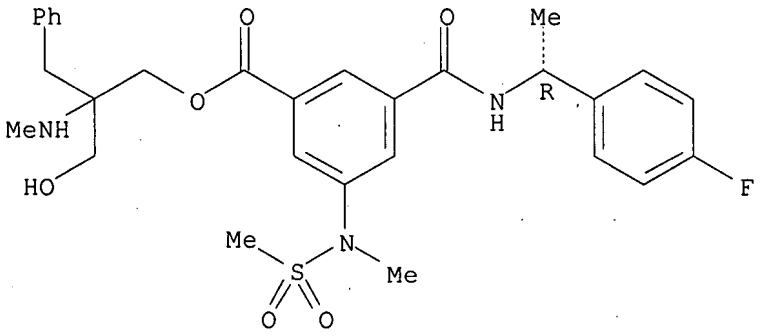
the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

IT 827039-49-6P 827039-50-9P 827039-51-0P
827039-52-1P 827039-53-2P 827039-54-3P
827039-55-4P 827039-56-5P 827039-60-1P
827039-61-2P 827039-65-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)

RN 827039-49-6 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester (9CI) (CA INDEX NAME)

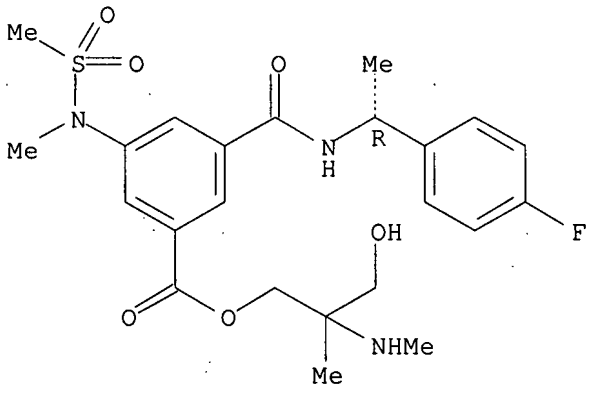
Absolute stereochemistry.



RN 827039-50-9 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-methyl-2-(methylamino)propyl ester (9CI) (CA INDEX NAME)

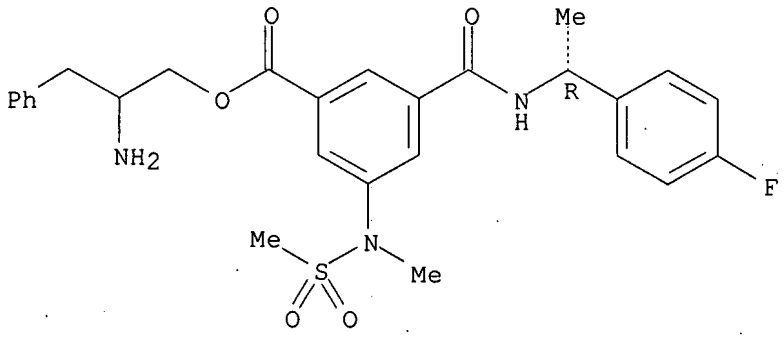
Absolute stereochemistry.



RN 827039-51-0 CAPLUS

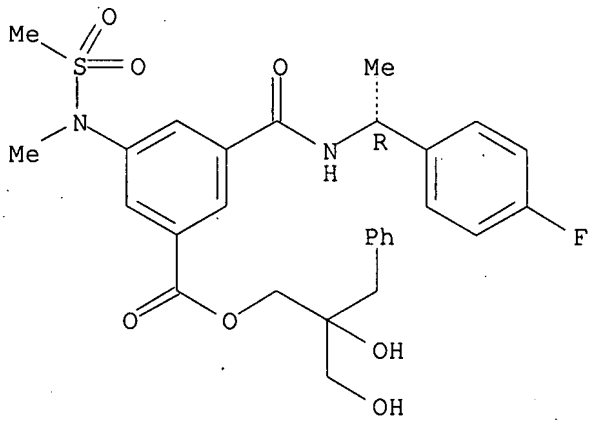
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-3-phenylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



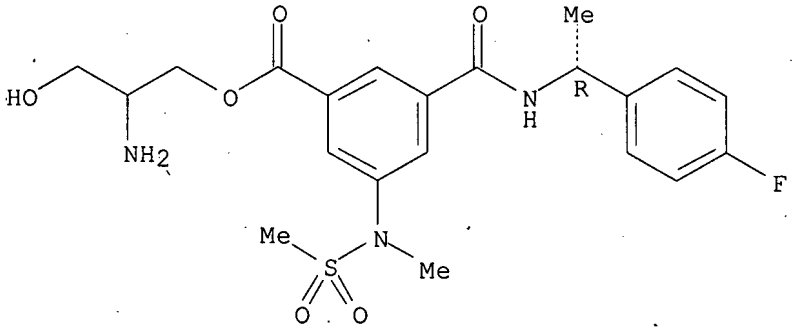
RN 827039-52-1 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2,3-dihydroxy-2-(phenylmethyl)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



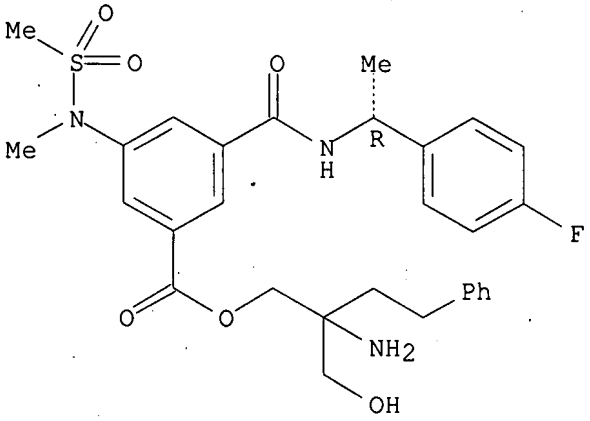
RN 827039-53-2 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-3-hydroxypropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



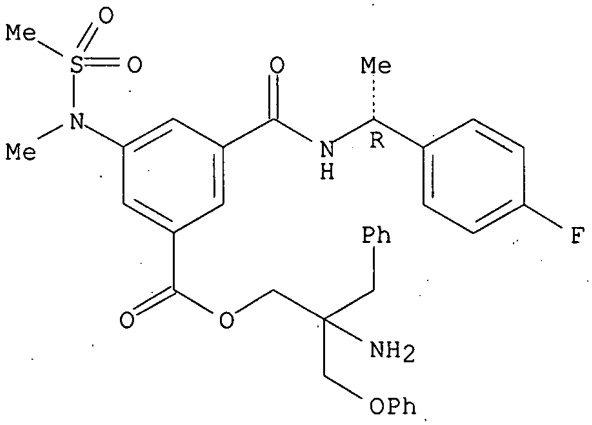
RN 827039-54-3 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-4-phenylbutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



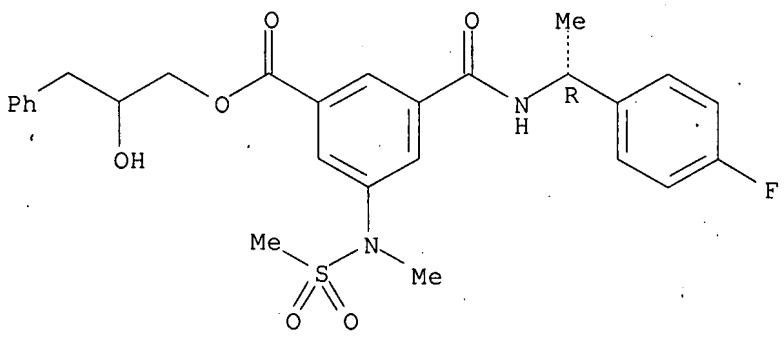
RN 827039-55-4 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(phenoxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



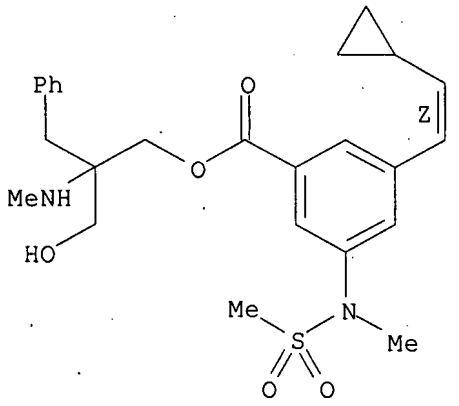
RN 827039-56-5 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-hydroxy-3-phenylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



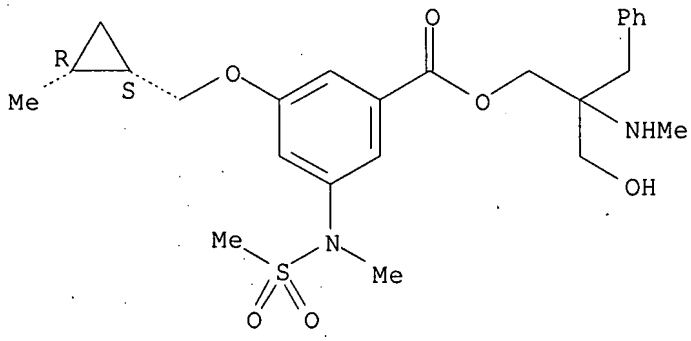
RN 827039-60-1 CAPLUS
CN Benzoic acid, 3-[(1Z)-2-cyclopropylethenyl]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester (9CI) (CA INDEX NAME)

Double bond geometry as shown.



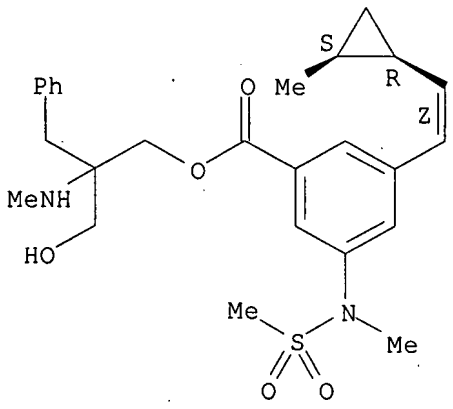
RN 827039-61-2 CAPLUS
CN Benzoic acid, 3-[[(1R,2S)-2-methylcyclopropyl]methoxy]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 827039-65-6 CAPLUS
CN Benzoic acid, 3-[(1Z)-2-[(1R,2S)-2-methylcyclopropyl]ethenyl]-5-[methyl(methylsulfonyl)amino]-, 3-hydroxy-2-(methylamino)-2-(phenylmethyl)propyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.



IT 827039-74-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)

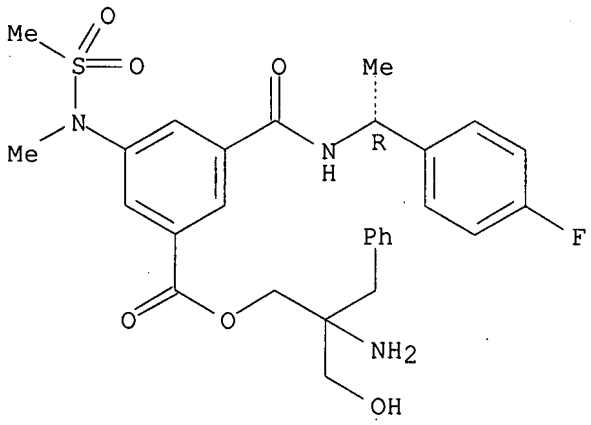
RN 827039-74-7 CAPLUS

CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

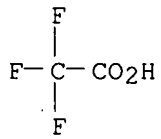
CRN 827039-73-6
CMF C28 H32 F N3 O6 S

Absolute stereochemistry.



CM 2

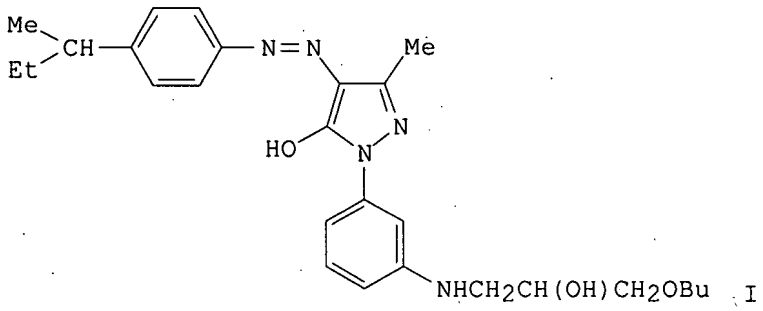
CRN 76-05-1
CMF C2 H F3 O2



L3 ANSWER 4 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1994:220382 CAPLUS
DN 120:220382
TI Liquid azo dyes and dye compositions and ink compositions using the same
IN Ono, Takashi; Yagyu, Tatsuya; Akase, Tetsumi
PA Orient Chemical Ind, Japan
SO Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 05311084	A	19931122	JP 1992-121882	19920514
	JP 2986609	B2	19991206		
	US 5326866	A	19940705	US 1993-59666	19930512
	EP 573809	A1	19931215	EP 1993-107875	19930514
	EP 573809	B1	19980819		
	R: CH, DE, FR, GB, LI				
PRAI	JP 1992-121882	A	19920514		

OS MARPAT 120:220382
GI



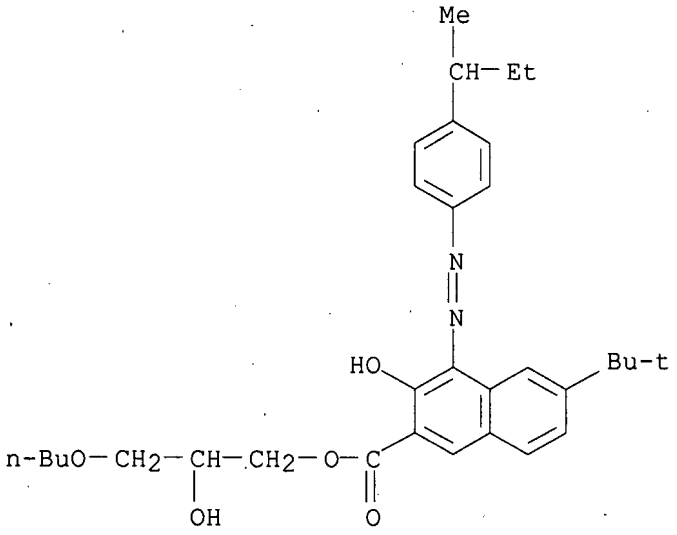
I

AB The title dyes soluble in alcs. and glycols are EtMeCHC6H4N:N(AN:N)nCpXCH2CH(OH)CH2OR [A = (un)substituted phenylene; n = 0, 1; Cp = pyrazolone derivative residue, naphthol derivative residue; X = NH, CO2; R = C3-12 alkyl]. 1-(3-Aminophenyl)-3-methyl-5-pyrazolone was treated with Bu glycidyl ether in diethanolamine at 80-85° for 8 h, and the product coupled with diazotized p-sec-butylaniline to obtain yellow I. A marking ink providing wet- and lightfast markings comprised I 7, EtOH 68, benzyl alc. 5, Et lactate 10, and phenolic resin 10 parts.

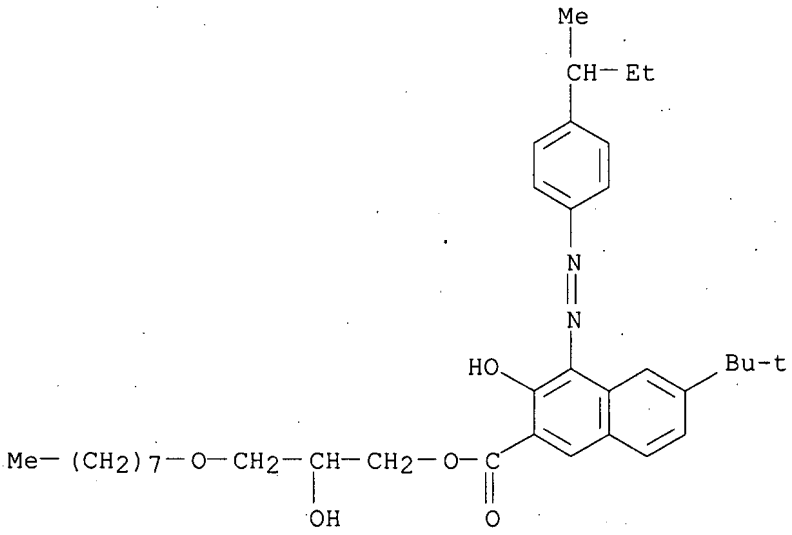
IT 154057-52-0P 154057-53-1P
RL: PREP (Preparation)
(manufacture of, dye, liquid, for inks)

RN 154057-52-0 CAPLUS

CN 2-Naphthalenecarboxylic acid, 6-(1,1-dimethylethyl)-3-hydroxy-4-[[4-(1-methylpropyl)phenyl]azo]-, 3-butoxy-2-hydroxypropyl ester (9CI) (CA INDEX NAME)



RN 154057-53-1 CAPLUS
CN 2-Naphthalenecarboxylic acid, 6-(1,1-dimethylethyl)-3-hydroxy-4-[[4-(1-methylpropyl)phenyl]azo]-, 2-hydroxy-3-(octyloxy)propyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 5 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1993:219790 CAPLUS
DN 118:219790
TI Thermal expansion of glassy polymers
AU Davy, K. W. M.; Braden, M.
CS Dent. Sch., Univ. London, London, E1 2AD, UK
SO Biomaterials (1992), 13(14), 1043-6
CODEN: BIMADU; ISSN: 0142-9612
DT Journal
LA English
AB The thermal expansion of a number of glassy polymers of interest in dentistry was studied using a quartz dilatometer. In some cases, the expansion was linear and therefore the coefficient of thermal expansion readily determined Other
polymers exhibited non-linear behavior and values appropriate to different

temperature ranges are quoted. The linear coefficient of thermal expansion was, to a
first approximation, a function of both the molar volume and van der Waal's volume
of the repeating unit.

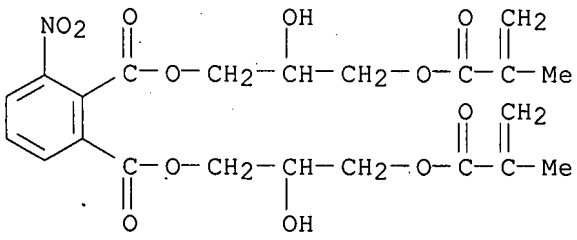
IT 147187-18-6
RL: PROC (Process)
(thermal expansion of, for dental materials)

RN 147187-18-6 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 3-nitro-, bis[2-hydroxy-3-[(2-methyl-1-oxo-2-propenyl)oxy]propyl] ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 147187-17-5
CMF C22 H25 N O12



L3 ANSWER 6 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1992:37119 CAPLUS
DN 116:37119
TI Hydroxyalkyl amino-substituted triiodobenzoates and addition polymers of triiodo compounds for x-ray contrast materials for the gastrointestinal tract
IN Sovak, Milos
PA USA
SO Can. Pat. Appl., 36 pp.
CODEN: CPXXEB
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CA 2031739	A1	19910609	CA 1990-2031739	19901207
	NO 9005299	A	19910610	NO 1990-5299	19901207
	EP 436316	A1	19910710	EP 1990-313363	19901207
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	AU 9067910	A	19910613	AU 1990-67910	19901210
	AU 637435	B2	19930527		
	JP 04208232	A	19920729	JP 1990-415693	19901210
PRAI	US 1989-448073	A	19891208		
	US 1990-574300	A	19900828		

OS MARPAT 116:37119

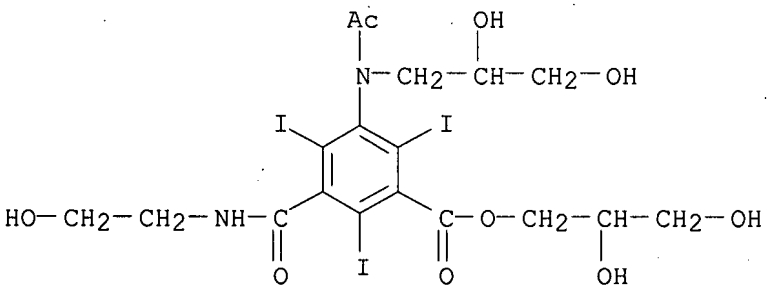
AB Hydroxyalkyl amino-substituted triiododbenzoates, wherein the remaining position is substituted with amino or carboxy, are provided. These compds. have low solubility in the gastrointestinal tract, but are resorbable from extravisceral body cavities and are useful as contrast media for the plain radiog. of the GI tract. Also, addition polymers comprising triiodo compds. bonded through an amino N to a nonoxocarbonyl group of an addition polymerizable monomer are provided. These polymers are water-soluble, physiol. acceptable agents useful for computer tomog. of the GI tract. A radiopaque water-soluble copolymer with low I content was prepared from acrylamide, 5-N-acrylamido-2,4,6-triidoisophthalic acid, and

N.N'-methylene-bis-acrylamide. The copolymer in water was treated with charcoal at 70-75° to remove monomers, filtered, diluted with an EDTA-containing solution, an autoclaved. The copolymer coated the gastrointestinal wall, was uniformly dispersed, gave no imaging artifacts, and delineated the entire tract with the same intensity of contrast throughout. The material also did not precipitate but seeped along the intestinal wall even in the presence of intestinal contents.

IT 138308-44-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as x-ray contrast agent for gastrointestinal tract imaging)

RN 138308-44-8 CAPLUS

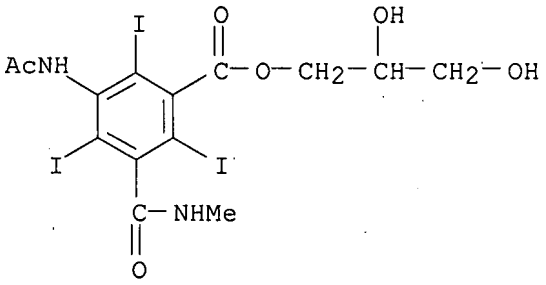
CN Benzoic acid, 3-[acetyl(2,3-dihydroxypropyl)amino]-5-[[(2-hydroxyethyl)amino]carbonyl]-2,4,6-triiodo-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



IT 138308-48-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, x-ray contrast agent for gastrointestinal tract imaging)

RN 138308-48-2 CAPLUS

CN Benzoic acid, 3-(acetylamino)-2,4,6-triiodo-5-[(methylamino)carbonyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 7 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1991:607264 CAPLUS

DN 115:207264

TI Synthesis and characterization of 1-methacryl-3-salicyloyl-2-hydroxypropane and its derivatives - a structure-reactivity kinetic study

AU Babu, N. Vijaya; Rajanna, K. C.; Rao, C. Janaki Ram

CS Nizam Coll., Osmania Univ., Hyderabad, 500 001, India

SO Proceedings - Indian Academy of Sciences, Chemical Sciences (1991), 103(4), 549-56
CODEN: PIAADM; ISSN: 0253-4134

DT Journal

LA English

OS CASREACT 115:207264

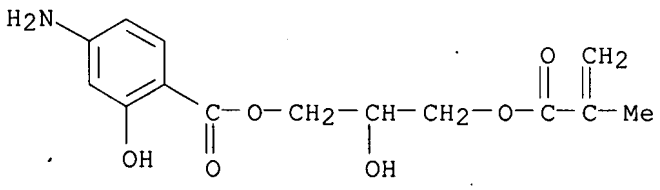
AB 2-HOC6H4CO2CH2CH(OH)CH2O2CCMe:CH2 (I) and its derivs. (Me, methoxy, Ac, thio, amino, chloro, and bromo) were prepared and characterized by elemental

anal., mass, IR, and 1H- and 13C-NMR spectroscopic results. I formation was 2nd order overall, 1st order each in salicylic acid and glycidyl methacrylate. A structural change (substituent change) in the salicylic acid changed its reactivity during I formation. Second-order rate consts. increase in the order 5-bromo < 5-chloro < Ac < H < thio < 4-amino < 4-Me < 4-chloro. Hammett's plot indicated a rho (ρ) value of 0.43. Deviation in the case of p-chloro substituent was explained in terms of resonance-interaction energy (ΔΔG) parameters. The effective sigma (.hivin.σ) value of p-chloro was 0.86, with ΔΔGp 1.274 cal/mol. The isokinetic temperature (β) is far below the exptl. temperature range (325-355 K), indicating the importance of entropy factors in controlling the reaction.

IT 136910-45-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 136910-45-7 CAPLUS

CN Benzoic acid, 4-amino-2-hydroxy-, 2-hydroxy-3-[(2-methyl-1-oxo-2-propenyl)oxy]propyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 8 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1991:460785 CAPLUS

DN 115:60785

TI Developer for electrostatography

IN Tsubushi, Kazuo; Kuramoto, Shinichi; Umemura, Kazuhiko; Takahashi, Toshihiko; Uematsu, Hidemi

PA Ricoh Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 02184865	A	19900719	JP 1989-5505	19890112
	JP 2849105	B2	19990120		
PRAI	JP 1989-5505		19890112		

AB The title developer contains a copolymer based on a monomer-containing dialkylaminobenzoic acid ester residue(s) or dialkylaminophthalic acid ester residue(s) and some other monomer. The developer (i.e. toner) gives copies with improved d., resolution, copy fixability, etc.

IT 135020-48-3D, copolymer with vinyl monomer
RL: USES (Uses)
(electrophotog. toner using)

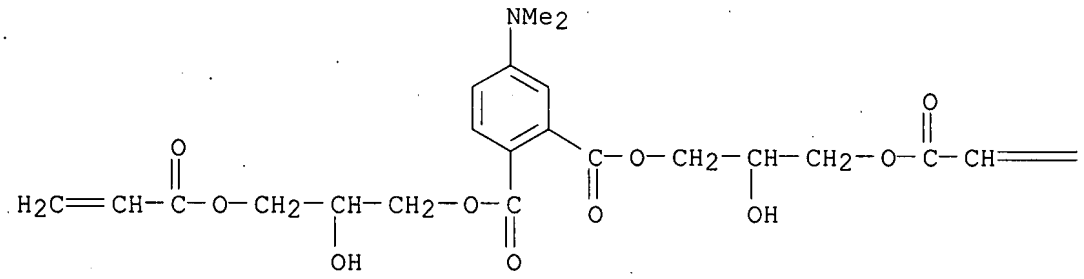
RN 135020-48-3 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4-(dimethylamino)-, bis[2-hydroxy-3-[(1-oxo-2-propenyl)oxy]propyl] ester, polymer with butyl 2-methyl-2-propenoate and ethyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 135020-47-2
CMF C22 H27 N O10

PAGE 1-A

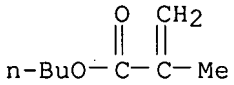


PAGE 1-B

$=CH_2$

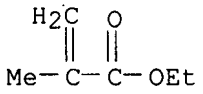
CM 2

CRN 97-88-1
CMF C8 H14 O2



CM 3

CRN 97-63-2
CMF C6 H10 O2



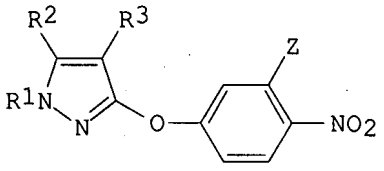
L3 ANSWER 9 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:423509 CAPLUS
DN 111:23509
TI Substituted 3-(4-nitrophenoxy)pyrazoles, their herbicidal use and compositions, and processes and intermediates for their preparation
IN Moedritzer, Kurt; Lee, Len Fang; Rogers, Michael David; Anderson, Dennis Keith; Singh, Rajendra Kumar; Gaede, Bruce John; Torrence, Lisa Louise
PA Monsanto Co., USA
SO Eur. Pat. Appl., 338 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

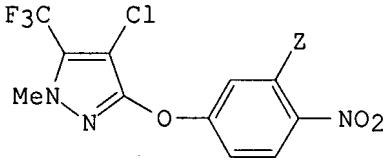
PI	EP 295233	A2	19881214	EP 1988-870104	19880607
	EP 295233	A3	19890315		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
	US 4855442	A	19890808	US 1988-175461	19880413
	US 4948902	A	19900814	US 1988-175462	19880413
	AU 8817450	A	19881208	AU 1988-17450	19880607
	AU 607225	B2	19910228		
	DK 8803086	A	19881209	DK 1988-3086	19880607
	FI 8802680	A	19881209	FI 1988-2680	19880607
	NO 8802509	A	19881209	NO 1988-2509	19880607
	NO 169387	B	19920309		
	NO 169387	C	19920617		
	BR 8802760	A	19881227	BR 1988-2760	19880607
	JP 01025764	A	19890127	JP 1988-140361	19880607
	JP 05075746	B	19931021		
	CN 1033457	A	19890621	CN 1988-103374	19880607
	CN 1021191	B	19930616		
	ZA 8804050	A	19900228	ZA 1988-4050	19880607
	HU 52063	A2	19900628	HU 1988-2946	19880607
	HU 204259	B	19911230		
	DD 289461	A5	19910502	DD 1988-316491	19880607
	PL 156831	B1	19920430	PL 1988-279591	19880607
	PL 156730	B1	19920430	PL 1988-279592	19880607
	PL 157154	B1	19920529	PL 1988-272883	19880607
	NO 8900595	A	19881209	NO 1989-595	19890210
	NO 170276	B	19920622		
	NO 170276	C	19920930		
	NO 8900596	A	19881209	NO 1989-596	19890210
	US 4964895	A	19901023	US 1990-471686	19900130
PRAI	US 1987-59431	A	19870608		
	US 1987-59712	A	19870608		
	US 1988-175460	A	19880413		
	US 1988-175461	A	19880413		
	US 1988-175462	A	19880413		
	US 1988-175463	A	19880413		
	NO 1988-2509	A1	19880607		

OS CASREACT 111:23509; MARPAT 111:23509

GI



I



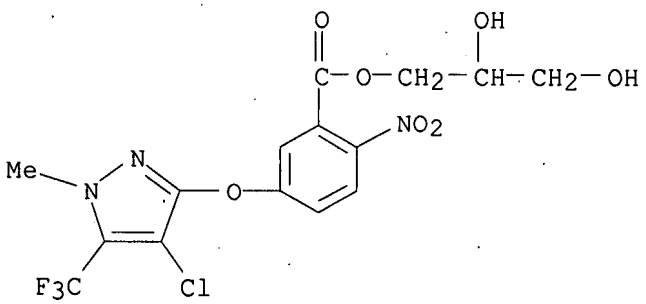
II

AB Title compds. I [R1 = Me, Et, halomethyl, haloethyl; R2 = Cl, cyano, halomethyl, haloethyl, MeS, EtS, MeS(O), EtS(O), MeS(O)2, EtS(O)2, MeOCH2; R3 = H, halo, NO2; Z = H, substituent of mol. weight ≤300] are prepared as herbicides. 3-Fluoroacetophenone underwent nitration by fuming HNO3 in the 6-position, followed by condensation with 5-trifluoromethyl-4-chloro-3-hydroxy-1-methylpyrazole to give (trifluoromethyl)chloro(nitrophenoxy)methylpyrazole II (Z = Ac). This underwent oximation by NH2OH.HCl, followed by etherification of the oxime with BrCH2CO2Me, to give II (Z = MeOCOCH2ON:CMe) (III). At 11.21 kg/ha postemergence, III gave 100% control of 9/10 tested weeds, including barnyardgrass, velvetleaf, and Pennsylvania smartweed.

IT 121303-65-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

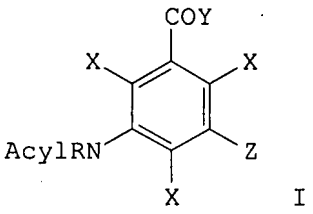
(preparation of, as herbicide)
RN 121303-65-9 CAPLUS
CN Benzoic acid, 5-[[4-chloro-1-methyl-5-(trifluoromethyl)-1H-pyrazol-3-yl]oxy]-2-nitro-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 10 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1989:192447 CAPLUS
DN 110:192447
TI Preparation of 5-acylamino-2,4,6-triiodo- or tribromobenzoic acid derivatives, useful as radiologic contrast imaging components
IN Felder, Ernest; Musu, Carlo; Fumagalli, Luciano; Uggeri, Fulvio
PA Bracco Industria Chimica S.p.A., Italy
SO PCT Int. Appl., 70 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 8809328	A1	19881201	WO 1988-EP453	19880520
	W: AU, BB, BG, BR, DK, FI, HU, JP, KP, KR, LK, MC, MG, MW, NO, RO, SD, SU, US				
	RW: AT, BE, BJ, CF, CG, CH, CM, DE, FR, GA, GB, IT, LU, ML, MR, NL, SE, SN, TD, TG				
	AU 8817978	A	19881221	AU 1988-17978	19880520
	AU 618535	B2	19920102		
	ZA 8803610	A	19890125	ZA 1988-3610	19880520
	ES 2006951	A6	19890516	ES 1988-1607	19880520
	EP 365541	A1	19900502	EP 1988-904526	19880520
	EP 365541	B1	19920812		
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
	JP 02503556	T	19901025	JP 1988-504455	19880520
	JP 2585087	B2	19970226		
	AT 79368	T	19920815	AT 1988-904526	19880520
	CA 1327600	C	19940308	CA 1988-567436	19880520
	IL 86450	A	19940530	IL 1988-86450	19880520
	US 5066823	A	19911119	US 1989-424216	19891010
PRAI	IT 1987-20647	A	19870522		
	IT 1988-47935	A	19880510		
	EP 1988-904526	A	19880520		
	WO 1988-EP453	A	19880520		

OS MARPAT 110:192447
GI



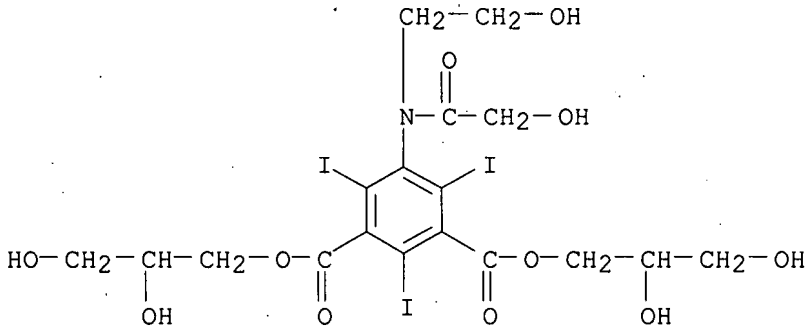
I

AB Title compds. I (X = Br, iodo; acyl = C2-6 hydroxyalkanoyl, alkoxyalkanoyl, alkoxyhydroxyalkanoyl, (un)substituted C2-4 alkanoyl; R = H, C1-6 alkyl, hydroxyalkyl, alkoxyalkyl, alkoxyhydroxyalkyl, H(OCH2CH2)2-5, Me(OCH2CH2)2-4, Et(OCH2CH2)2-4, alkylene analog of I; Y = HO, alkoxy, hydroxyalkoxy, alkylamino, etc.; Z = COY, hydroxyalkylaminocarbonyl, C2-5 acylamino, hydroxyacylamino, N-alkylacylamino, N-hydroxyalkylacylamino, acylaminomethyl), components of contrast agents in radiol. (no data) are prepared S-5-(1-Methylaminocarbonylethoxy)-2,4,6-triiodobis(1,3-dihydroxyisopropyl)isophthalamide in DMF was reacted with MeONa/MeOH at room temperature to give 70.4% I [Y = (HOCH2)2CHNH, Z = (HOCH2)2CHNHCO, acyl = MeCH(OH)COCH2, R = H, X = iodo).

IT 120396-61-4P 120396-63-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as radiocontrast agent)

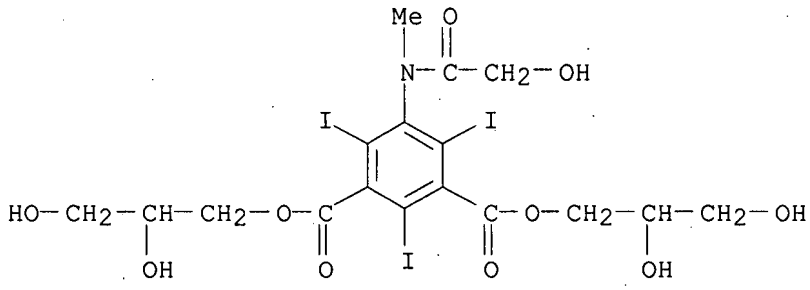
RN 120396-61-4 CAPLUS

CN 1,3-Benzenedicarboxylic acid, 5-[(hydroxyacetyl)(2-hydroxyethyl)amino]-2,4,6-triiodo-, bis(2,3-dihydroxypropyl) ester (9CI) (CA INDEX NAME)



RN 120396-63-6 CAPLUS

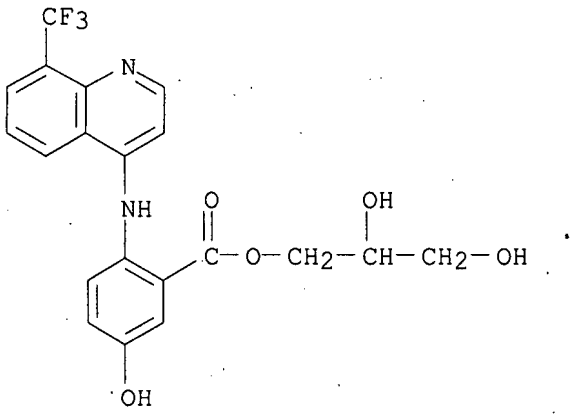
CN 1,3-Benzenedicarboxylic acid, 5-[(hydroxyacetyl)methylamino]-2,4,6-triiodo-, bis(2,3-dihydroxypropyl) ester (9CI) (CA INDEX NAME)



L3 ANSWER 11 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1989:127904 CAPLUS

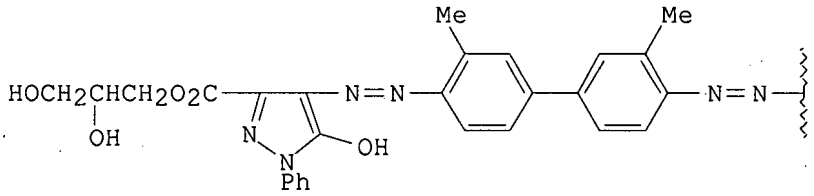
DN 110:127904
TI Simultaneous determination of plasma floctafenin and its major metabolites by high-performance liquid chromatography: preliminary observations in children
AU Nicot, G.; Lachatre, G.; Terrier, G.; Gonnet, C.; Rocca, J. L.; Desroches, R.; Lansade, A.
CS Cent. Hosp. Reg., Univ. Hop. Dupuytren, Limoges, 87042, Fr.
SO Therapeutic Drug Monitoring (1989), 11(1), 67-72
CODEN: TDMODV; ISSN: 0163-4356
DT Journal
LA English
AB An isocratic reversed-phase ion-pair liquid chromatog. with UV detection at 350 nm for the determination in human plasma of floctafenin (F) and its 3 main metabolites [floctafenic acid (FA), hydroxyfloctafenin (HOF), and hydroxyfloctafenic acid (HOFA)] is reported. Analytes and internal standard were extracted from acidified plasma into EtOAc, and this organic phase was evaporated to dryness. This extraction yielded plasma drug recoveries of >72%. With 1 mL of plasma, the lower quantification limit was 0.05 μg/mL with excellent linearity up to 0.8 μg/mL for HOF and HOFA and up to 4.0 μg/mL for F and FA. The reproducibility and the selectivity of the method in the presence of several drugs thought likely to be administered in conjunction with F were demonstrated. This method was successfully applied to a pharmacokinetic study with a single 10-mg/kg oral dose in children.
IT 56047-11-1
RL: ANT (Analyte); ANST (Analytical study)
(determination of, as floctafenin metabolite, in blood of children by HPLC)
RN 56047-11-1 CAPLUS
CN Benzoic acid, 5-hydroxy-2-[[8-(trifluoromethyl)-4-quinolinyl]amino]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)

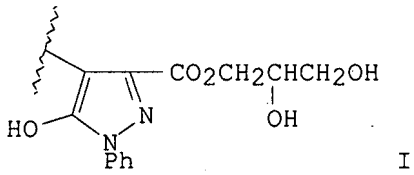


L3 ANSWER 12 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1988:530818 CAPLUS
DN 109:130818
TI Alcohol-soluble dye compositions
IN Ono, Takashi; Ikegami, Akiko
PA Orient Chemical Industries, Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 63075068	A	19880405	JP 1986-221165	19860918

JP 06094546 B 19941124
PRAI JP 1986-221165 19860918
OS MARPAT 109:130818
GI





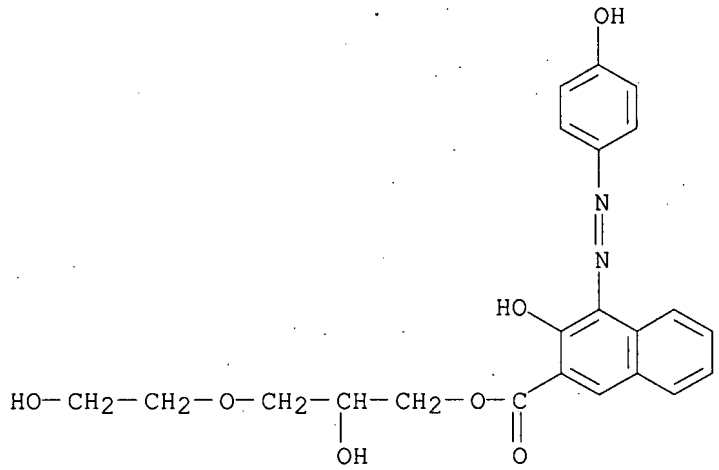
I

AB Dye compns., soluble in lower alcs. such as PrOH, BuOH, and propylene glycol monoalkyl ethers and useful for marking inks, comprise reaction mixts. obtained by treating dyes or their precursors containing active H connected to N or O and no other type of active H with epoxy compds. and converting the precursors to dyes. The reaction mixts. may contain compds. Dm[CH2CH(OH)R]n [D = dye residue; R = C1-4 alkyl, CH2OR1; R1 = H, C1-5 alkyl, C1-5 alkenyl, (meth)acryloyl, CH2CH2CH2Si(OMe)3, polyol residue with mol. weight ≤300; m = 1-2; n = 1-4]. Thus, 0.2 mol 1-phenyl-3-carboxy-5-pyrazolone was treated with 0.6 mol glycidol and triethanolamine (catalyst) in H2O at 80-85° and the product was coupled with 0.1 mol diazotized o-tolidine at 10-15° to give dye I. A 20% PrOH solution of I was stable when kept at -5 or +60° for 3 mo.

IT 116429-92-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of, alc.-soluble, for marking inks)

RN 116429-92-6 CAPLUS

CN 2-Naphthalenecarboxylic acid, 3-hydroxy-4-[(4-hydroxyphenyl)azo]-, 2-hydroxy-3-(2-hydroxyethoxy)propyl ester (9CI) (CA INDEX NAME)

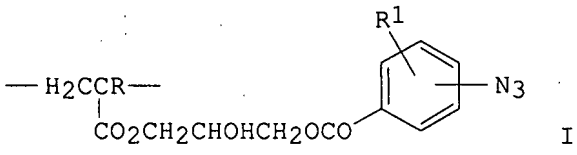


L3 ANSWER 13 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1987:468173 CAPLUS
DN 107:68173
TI Negative-working photoresist
IN Goto, Yoshitaka; Yazawa, Toshiya; Fujii, Kenichi; Yamada, Eiichi
PA Nippon Oils & Fats Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 61239245	A	19861024	JP 1985-80090	19850417
PRAI	JP 1985-80090		19850417		

GI



I

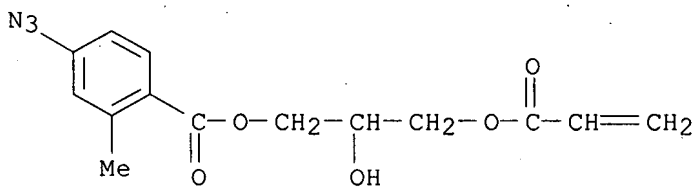
AB The photosensitive component of the photoresist is a polymer having mol. weight ≥5000 and repeating units I (R = H, C1-2 alkyl; R1 = H, C1-3 alkyl, C1-3 alkoxy). The polymer has high photosensitivity and acid resistance and is storage stable. Thus, 2-hydroxy-3-azidobenzoyloxypropyl methacrylate 45, Et acrylate 30, benzyl methacrylate 25, tert-butyl 2-ethylperoxyhexanoate 1 parts and MEK were made to react at 80° for 5 h to give a polymer having mol. weight 75,000 after purification A solution containing the polymer and 5-nitroacenaphthene (10% weight of the polymer) was used to form a 2-μ layer on a Cu substrate. The material was sensitometrically exposed to a Hg lamp, developed with trichloroethylene, and etched with FeCl3. Sensitivity was much higher than controls using poly(vinyl cinnamate) with or without a sensitizer or a similar polymer but having mol. weight 3500. The controls also showed inferior stabilities.

IT 109180-29-2 109180-31-6
RL: TEM (Technical or engineered material use); USES (Uses)
(photoresist composition containing, for improved stability)

RN 109180-29-2 CAPLUS
CN 2-Butenedioic acid (2Z)-, dimethyl ester, polymer with ethenyl acetate and 2-hydroxy-3-[(1-oxo-2-propenyl)oxy]propyl 4-azido-2-methylbenzoate (9CI) (CA INDEX NAME)

CM 1

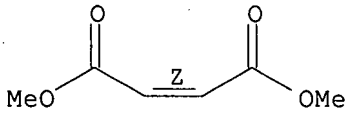
CRN 109180-28-1
CMF C14 H15 N3 O5



CM 2

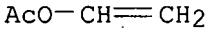
CRN 624-48-6
CMF C6 H8 O4

Double bond geometry as shown.



CM 3

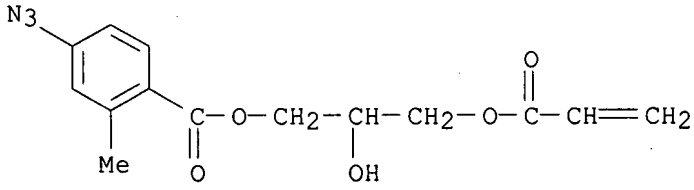
CRN 108-05-4
CMF C4 H6 O2



RN 109180-31-6 CAPLUS
CN Benzoic acid, 4-azido-2-methyl-, 2-hydroxy-3-[(1-oxo-2-propenyl)oxy]propyl ester, polymer with ethenylbenzene and methyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

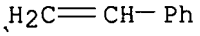
CM 1

CRN 109180-28-1
CMF C14 H15 N3 O5



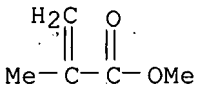
CM 2

CRN 100-42-5
CMF C8 H8



CM 3

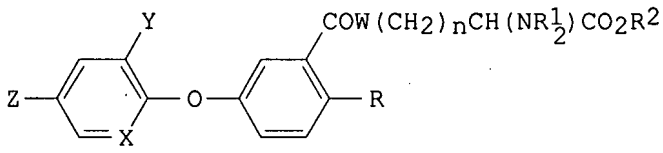
CRN 80-62-6
CMF C5 H8 O2



L3 ANSWER 14 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1986:621000 CAPLUS
DN 105:221000
TI Substituted aryloxybenzoyl amino acid herbicides and methods of use
IN Nagubandi, Sreeramulu
PA Stauffer Chemical Co., USA
SO U.S., 6 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4602946	A	19860729	US 1985-704815	19850225
PRAI	US 1985-704815		19850225		

OS MARPAT 105:221000
GI

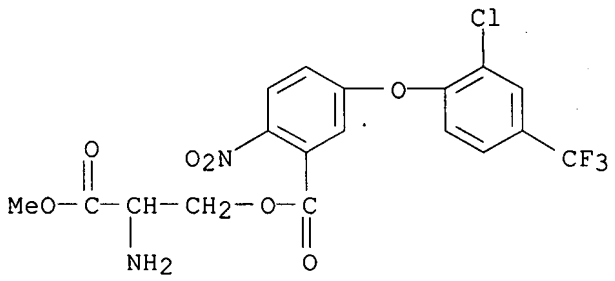


I

AB The title compound I (R = NO2, H, halo; R1 = H, C1-6 alkyl, SCCl3 etc.; R2 = C1-8 alkyl, H, aryl, Mg, Ca, Ba, Fe, Cu, Zn, etc.; n = 1-4; W = O, S, NH; X = CH, N; Y = Cl, Br, F, iodo, Me, H, CN; Z = H, Cl, Br, iodo, F or CHmF3-m; m = 0-3) are prepared as herbicides. Thus, 79.0 g 2-nitro-5-[(2-chloro-4-trifluoromethyl)phenoxy]benzoyl chloride was reacted with 1.50 g DL-serine Me ester-HCl for 15-25 h to give I (R = NO2, R1 = H, R2 = Me, W = O, n = 1, X = CH, Y = Cl, Z = CF3) (II). Postemergence II, applied at 0.25 lb/acre, totally controlled foxtail (Setaria), hemp sesbania (Sesbania exaltala), nightshade (Solanum) and sorghum (Sorghum bicolor) in flats.

IT 105388-01-0P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

RN 105388-01-0 CAPLUS
CN Serine, methyl ester, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitrobenzoate (ester) (9CI) (CA INDEX NAME)

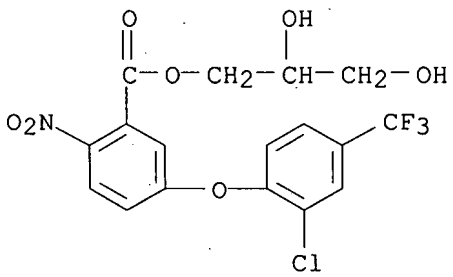


L3 ANSWER 15 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1983:160411 CAPLUS
DN 98:160411
TI Phenoxybenzoates, compositions containing them and their use
IN Liu, Kou Chang; Brown, Michael J.
PA GAF Corp., USA
SO Eur. Pat. Appl., 96 pp.
CODEN: EPXXDW
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 66106	A1	19821208	EP 1982-103897	19820505
	R: BE, DE, FR, GB, IT				
	US 4435588	A	19840306	US 1981-283402	19810715
	US 4797505	A	19890110	US 1982-358974	19820317
	ZA 8203288	A	19831228	ZA 1982-3288	19820512
	ES 512427	A1	19830201	ES 1982-512427	19820521
	BR 8202970	A	19830503	BR 1982-2970	19820521
	JP 58010540	A	19830121	JP 1982-85702	19820522
	US 4568382	A	19860204	US 1983-557570	19831202
PRAI	US 1981-266675	A	19810522		
	US 1981-283402	A	19810715		
	US 1981-292320	A	19810812		
	US 1981-301664	A	19810914		
	US 1981-310663	A	19811013		
	US 1982-358974	A	19820317		

OS CASREACT 98:160411; MARPAT 98:160411
AB Seventy herbicidal phenoxybenzoates 2,5-R(R1O)C6H3COR2 (I, R = NO2, cyano, amino; R1 = substituted Ph; R2 = esterified OH, SH, amino) were prepared by various methods. Thus, 448.1 g I [R = NO2, R1 = 2,4-Cl(F3C)C6H3, R2 = OH] was treated with 458 g SOCl2 to give 282.9 g acid chloride (II). II, (15 g) reacted with 10 g (HOCH2CH2S)2 to give 7.7 g I [R = NO2, R1 = 2,4-Cl(F3C)C6H3, R2 = OCH2CH2SSCH2CH2OH] (III). Applied both pre- and post-emergence, 10 lb III/acre gave complete kill of e.g. morning glory, with little effect on crop plants.
IT 85300-90-9P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and herbicidal activity of)
RN 85300-90-9 CAPLUS
CN Benzoic acid, 5-[2-chloro-4-(trifluoromethyl)phenoxy]-2-nitro-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 16 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1981:587045 CAPLUS
DN 95:187045
TI Benzoyl derivatives and their pharmaceutical use
IN Keck, Johannes; Krueger, Gerd; Pieper, Helmut; Noll, Klaus; Engelhardt,

Guenther; Promberger, Norbert; Zimmermann, Rainer
PA Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger.
SO Ger. Offen., 111 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2926472	A1	19810115	DE 1979-2926472	19790630
	EP 24282	A1	19810304	EP 1980-103099	19800604
	EP 24282	B1	19830518		
	R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	AT 3415	T	19830615	AT 1980-103099	19800604
	JP 56010155	A	19810202	JP 1980-78281	19800610
	US 4362738	A	19821207	US 1980-158587	19800611
	DK 8002794	A	19801231	DK 1980-2794	19800627
	FI 8002049	A	19801231	FI 1980-2049	19800627
	NO 8001931	A	19810102	NO 1980-1931	19800627
	AU 8059735	A	19810205	AU 1980-59735	19800627
	AU 538776	B2	19840830		
	ES 492845	A1	19811101	ES 1980-492845	19800627
	IL 60418	A	19840229	IL 1980-60418	19800627
	ZA 8003907	A	19820224	ZA 1980-3907	19800630
	CA 1140564	A1	19830201	CA 1980-355151	19800630
PRAI	DE 1979-2926472	A	19790630		
	EP 1980-103099	A	19800604		

OS MARPAT 95:187045
GI

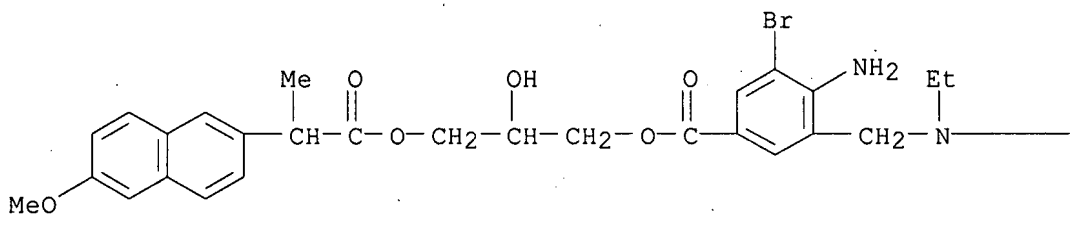
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

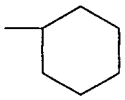
AB Title compds. I [R, R1 = H, alkyl, optionally substituted Ph; RR1 = alkylene, (CH2CH2)2N; R2 = H, F, Cl, Br; R3 = acyl; X = O, NH; X1 = cycloalkylene, alkylene, carbalkoxy] were prepared Thus, II.HCl was stirred with III overnight to give IV. IV had an ED35 = 84.7 mg/kg (s.c.) in the carrageenin edema test.

IT 78436-58-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(deacetylation of)

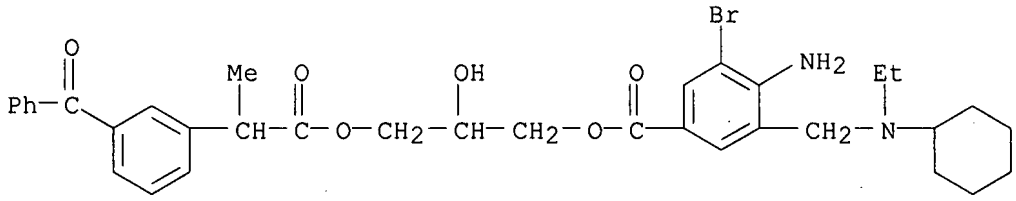
RN 78436-58-5 CAPLUS
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



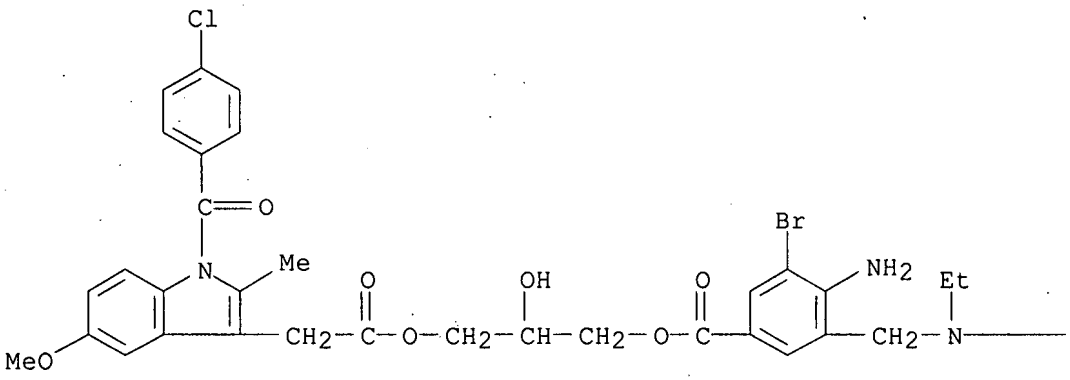


IT 78436-49-4P 78436-53-0P 78436-58-5P
78436-60-9P 78436-64-3P 78458-40-9P
78458-47-6P 78458-48-7P 78458-49-8P
78458-50-1P 78458-51-2P 78458-53-4P
78458-55-6P 78480-99-6P 78481-00-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 78436-49-4 CAPLUS
CN Benzeneacetic acid, 3-benzoyl-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester, monohydrochloride (9CI) (CA INDEX NAME)

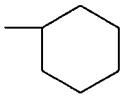


● HCl

RN 78436-53-0 CAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester (9CI) (CA INDEX NAME)

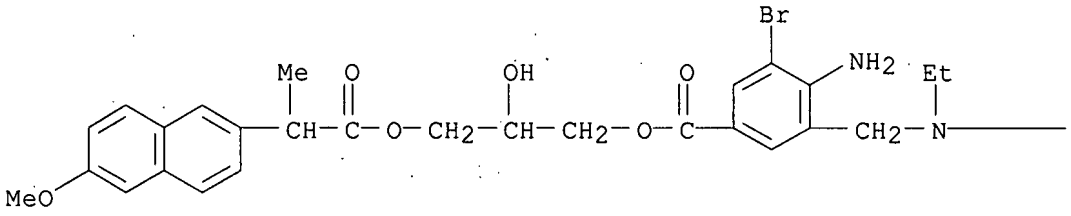


PAGE 1-B

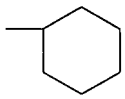


RN 78436-58-5 CAPLUS
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



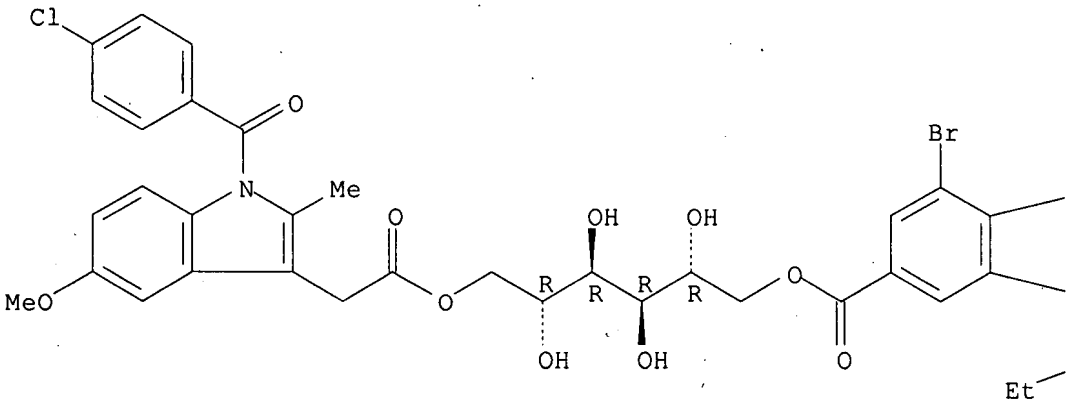
PAGE 1-B



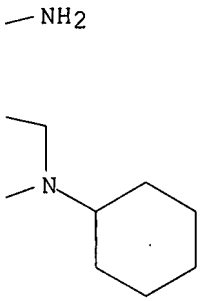
RN 78436-60-9 CAPLUS
CN D-Mannitol, 1-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate] 6-[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

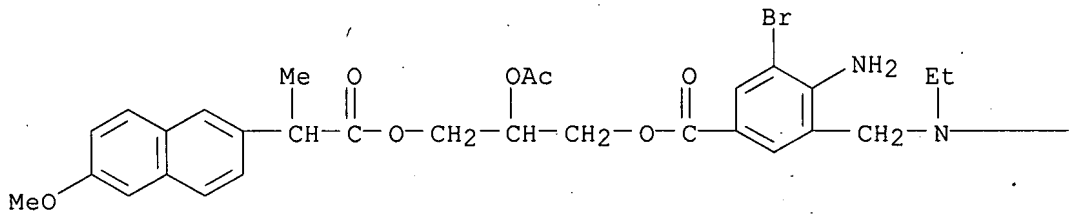


PAGE 1-B

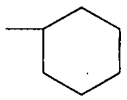


RN 78436-64-3 CAPLUS
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2-(acetyloxy)-3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A

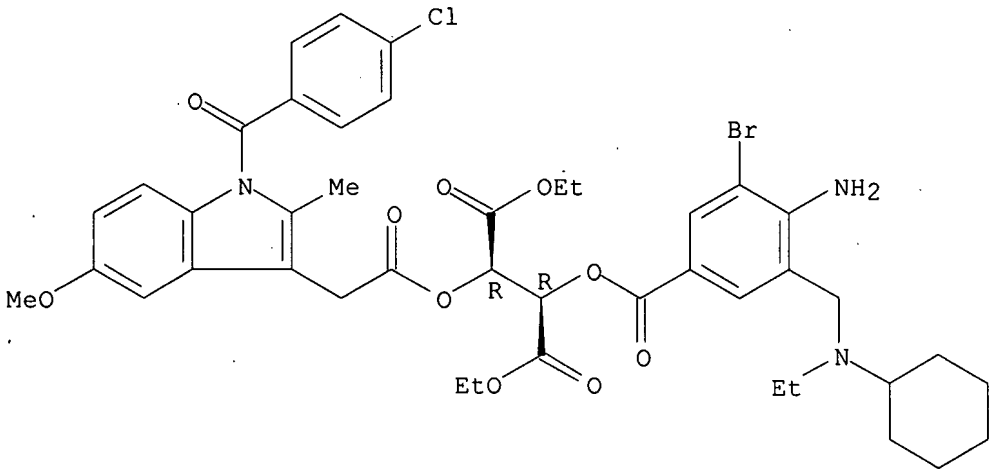


● HCl

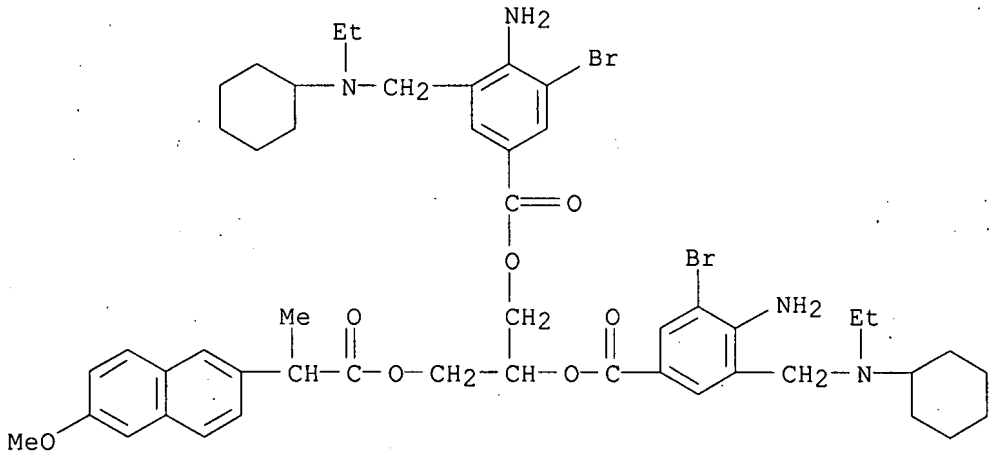


RN 78458-40-9 CAPLUS
CN Butanedioic acid, 2-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-3-[[[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl]acetyl]oxy]-, diethyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

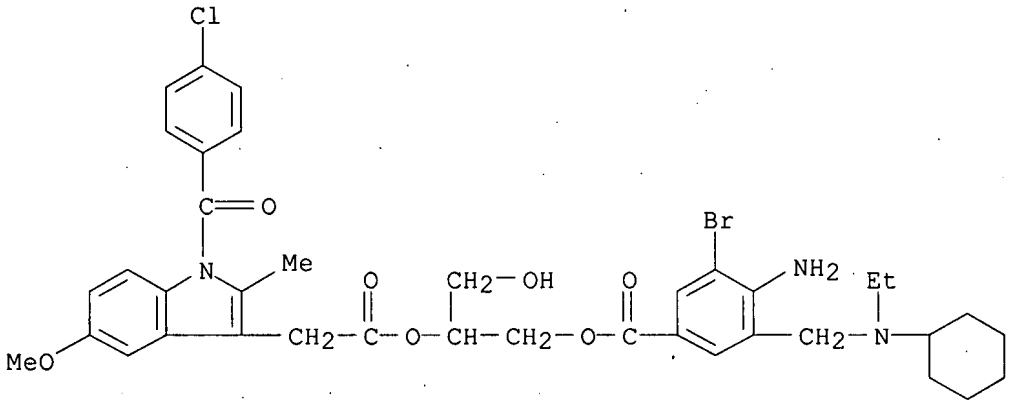


RN 78458-47-6 CAPLUS
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 2,3-bis[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]propyl ester (9CI) (CA INDEX NAME)



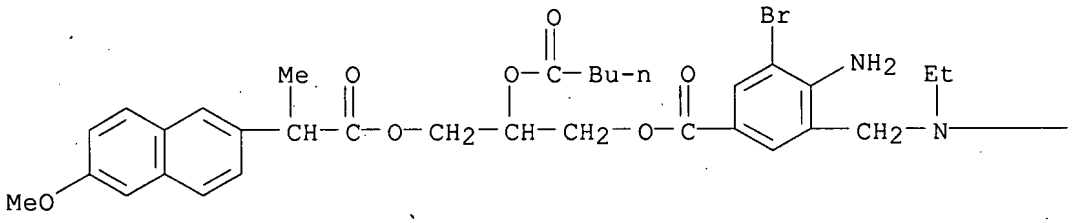
RN 78458-48-7 CAPLUS
CN 1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-, 2-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-1-

(hydroxymethyl)ethyl ester (9CI) (CA INDEX NAME)



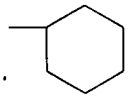
RN 78458-49-8 CAPLUS
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-[(1-oxopentyl)oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



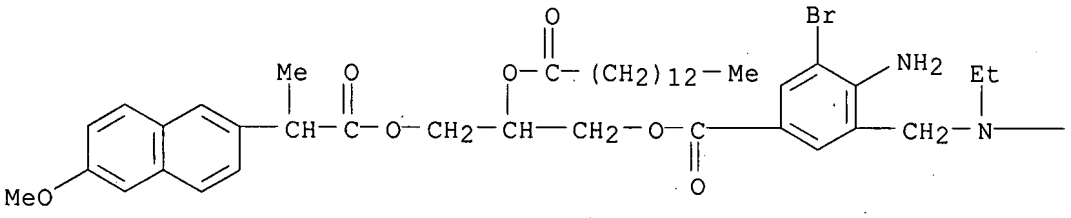
● HCl

PAGE 1-B



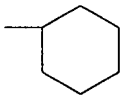
RN 78458-50-1 CAPLUS
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-[(1-oxotetradecyl)oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



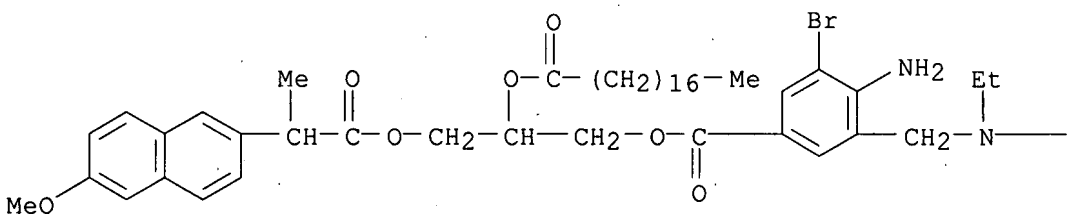
● HCl

PAGE 1-B



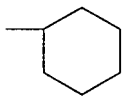
RN 78458-51-2 CAPLUS
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-[(1-oxooctadecyl)oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



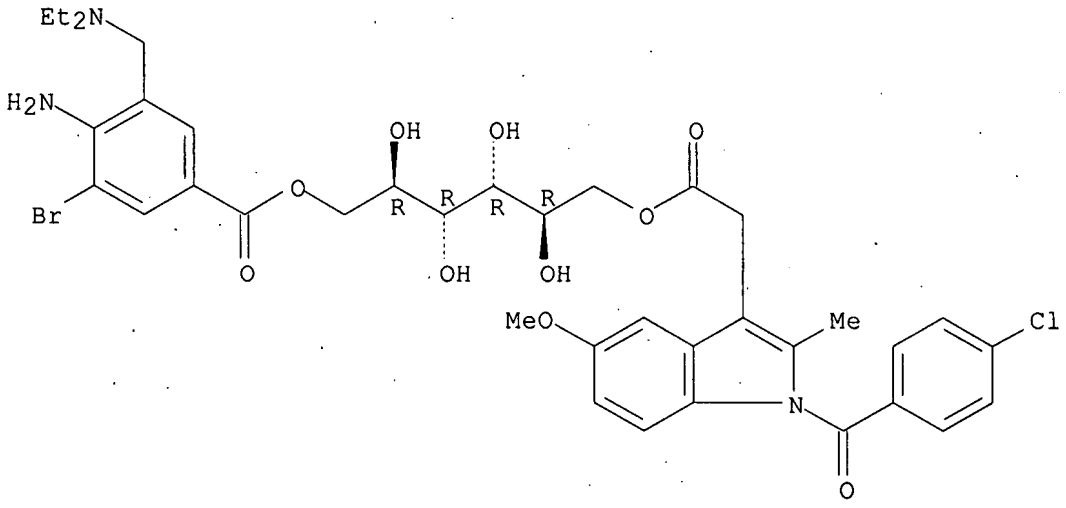
● HCl

PAGE 1-B



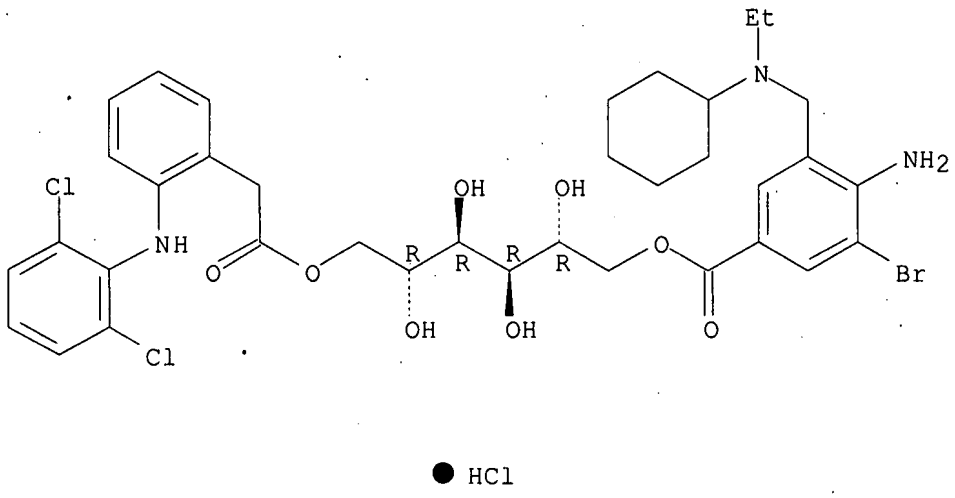
RN 78458-53-4 CAPLUS
CN D-Mannitol, 1-[4-amino-3-bromo-5-[(diethylamino)methyl]benzoate] 6-[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



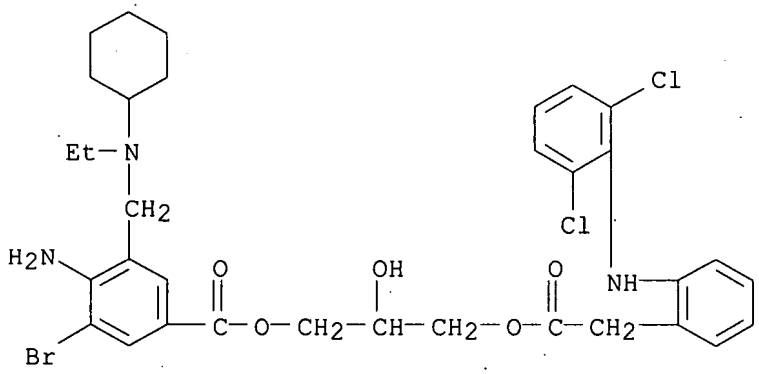
RN 78458-55-6 CAPLUS
CN D-Mannitol, 1-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate] 6-[2-[(2,6-dichlorophenyl)amino]benzeneacetate], monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

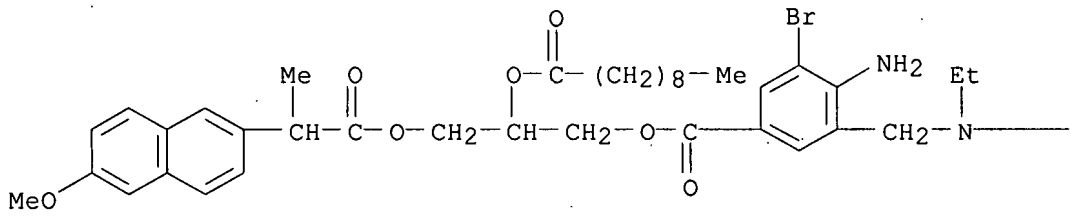
RN 78480-99-6 CAPLUS
CN Benzeneacetic acid, 2-[(2,6-dichlorophenyl)amino]-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-hydroxypropyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

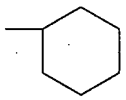
RN 78481-00-2 CAPLUS
CN 2-Naphthaleneacetic acid, 6-methoxy-α-methyl-, 3-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-2-[(1-oxodecyl)oxy]propyl ester, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



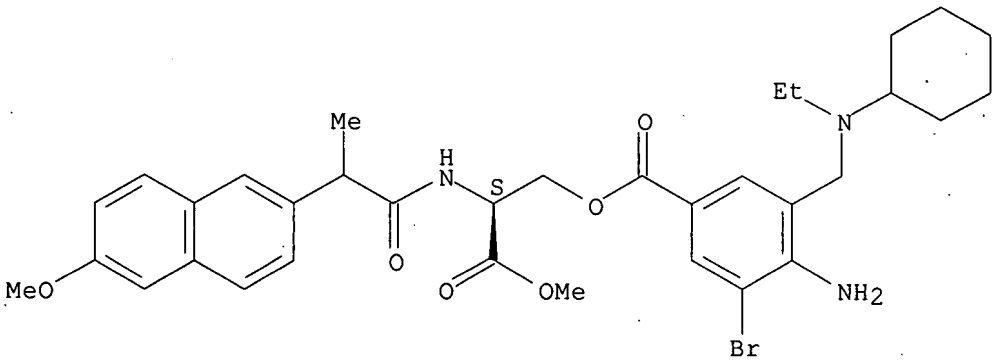
● HCl

PAGE 1-B



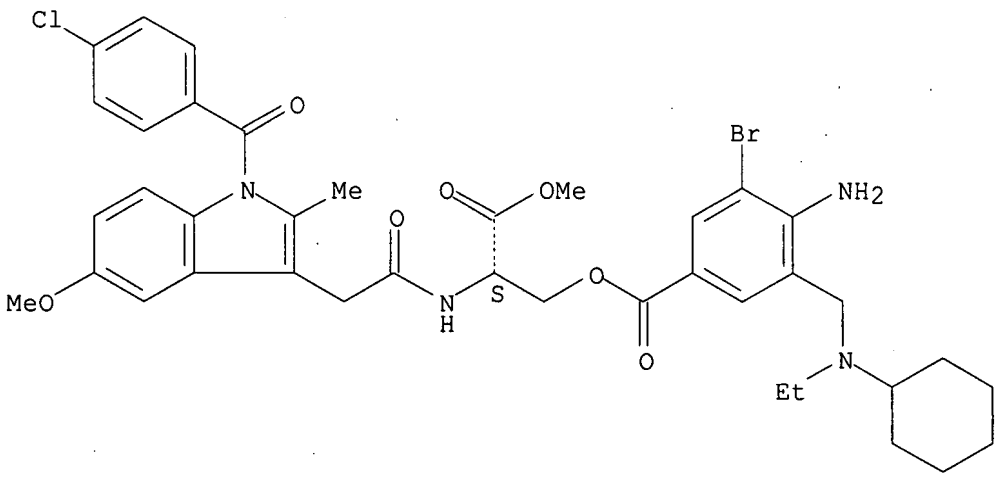
IT 78436-55-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with indoleacetic acid imidazolide)
RN 78436-55-2 CAPLUS
CN L-Serine, N-[2-(6-methoxy-2-naphthalenyl)-1-oxopropyl]-, methyl ester, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

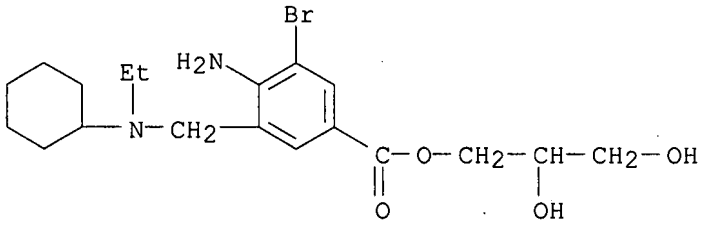


IT 78458-83-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with naphthaleneacetic acid imidazolide)
RN 78458-83-0 CAPLUS
CN L-Serine, N-[[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indol-3-yl]acetyl]-, methyl ester, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate (ester) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



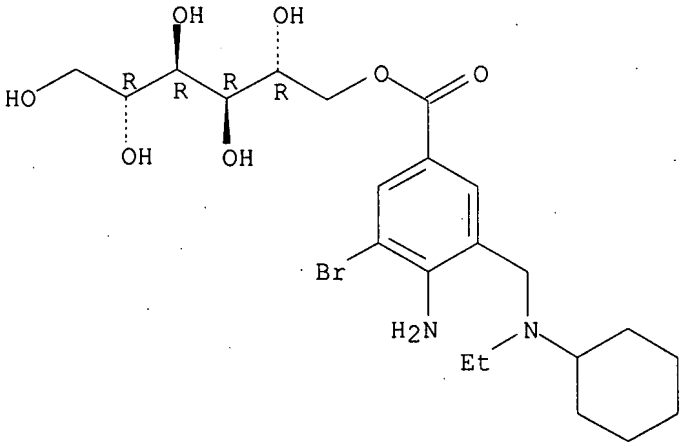
IT 78412-77-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetic acid imidazolide derivative)
RN 78412-77-8 CAPLUS
CN Benzoic acid, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



IT 78458-54-5
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with phenylaminophenylacetic acid)
RN 78458-54-5 CAPLUS
CN D-Mannitol, 1-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate] (9CI) (CA INDEX NAME)

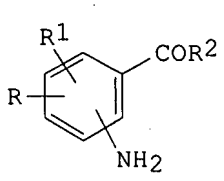
Absolute stereochemistry.



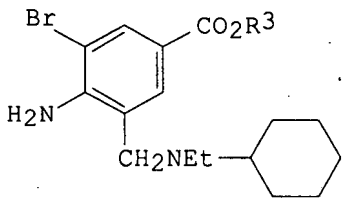
L3 ANSWER 17 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1981:461792 CAPLUS
DN 95:61792
TI Aminobenzoic acid derivatives for use as pharmaceuticals or intermediate products
IN Noll, Klaus; Keck, Johannes; Pieper, Helmut; Krueger, Gerd; Ballhause, Helmut; Bauer, Eckhart
PA Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger.
SO Ger. Offen., 60 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2926471	A1	19810115	DE 1979-2926471	19790630
	JP 56010154	A	19810202	JP 1980-78280	19800610
	AT 8003063	A	19820715	AT 1980-3063	19800611
	AT 370085	B	19830225		
	DK 8002793	A	19801231	DK 1980-2793	19800627
	FI 8002048	A	19801231	FI 1980-2048	19800627
	NO 8001930	A	19810102	NO 1980-1930	19800627
	ES 492843	A1	19811116	ES 1980-492843	19800627
	CA 1140934	A1	19830208	CA 1980-355165	19800630
PRAI	DE 1979-2926471	A	19790630		

OS MARPAT 95:61792
GI



I



II

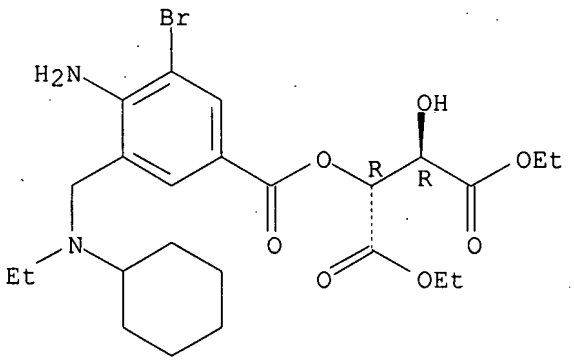
AB Aminobenzoates I (R = aminomethyl; R1 = H, F, Cl, Br; R2 = esterified OH, substituted NH2) were prepared Thus II (R3 = Na) was treated with chloropropanediol to give II [R3 = CH2CH(OH)CH2OH](III). At 100 mg/kg orally in rats III caused 89% inhibition of gastric erosion induced by EtOH.

IT 78412-80-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antiulcer activity of)

RN 78412-80-3 CAPLUS

CN Butanedioic acid, 2-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-3-hydroxy-, diethyl ester, monohydrochloride, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



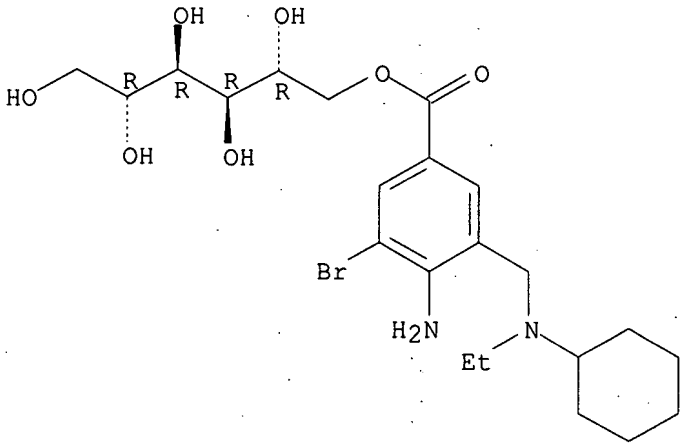
● HCl

IT 78411-95-7P 78412-81-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antiulcer activity of)

RN 78411-95-7 CAPLUS

CN D-Mannitol, 1-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate], monohydrochloride (9CI) (CA INDEX NAME)

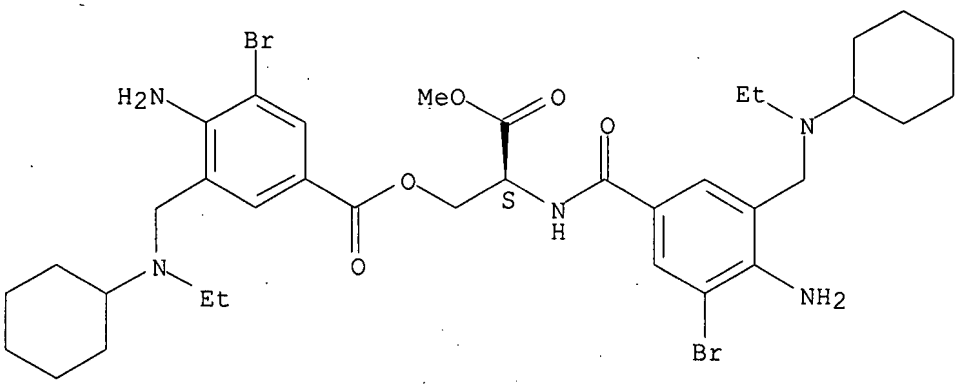
Absolute stereochemistry.



● HCl

RN 78412-81-4 CAPLUS
CN L-Serine, N-[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]-, methyl ester, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate (ester) (9CI) (CA INDEX NAME)

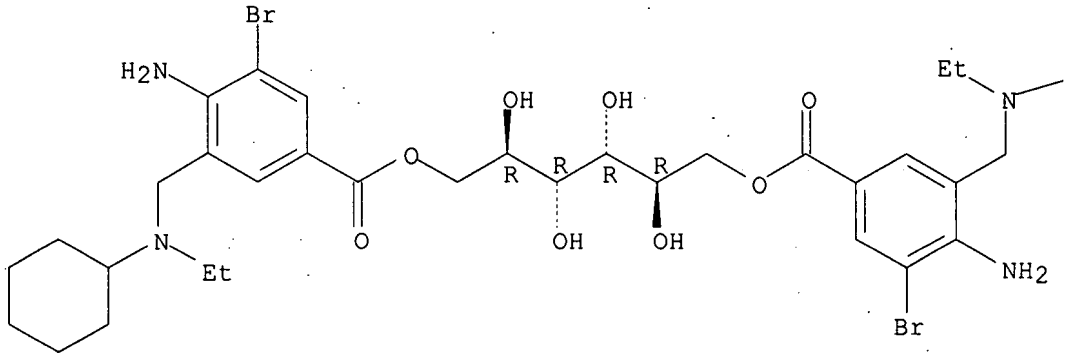
Absolute stereochemistry.



IT 78411-94-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 78411-94-6 CAPLUS
CN D-Mannitol, 1,6-bis[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoate], dihydrochloride (9CI) (CA INDEX NAME)

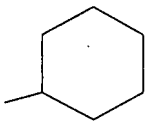
Absolute stereochemistry.

PAGE 1-A



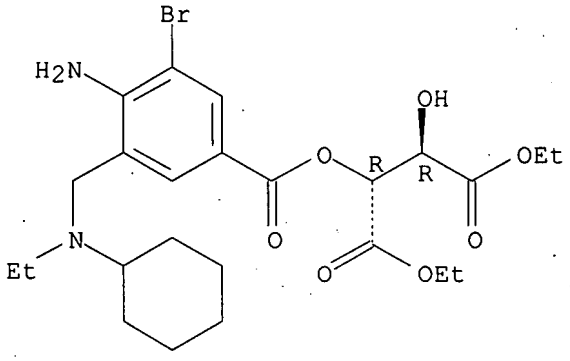
●2 HCl

PAGE 1-B

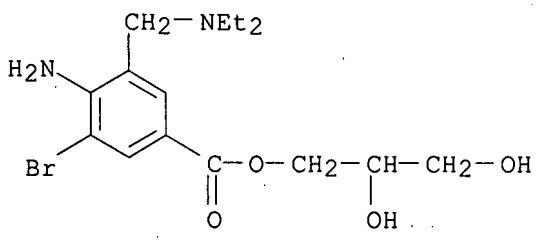


IT 78412-12-1P 78412-42-7P 78412-77-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 78412-12-1 CAPLUS
CN Butanedioic acid, 2-[[4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]benzoyl]oxy]-3-hydroxy-, diethyl ester, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

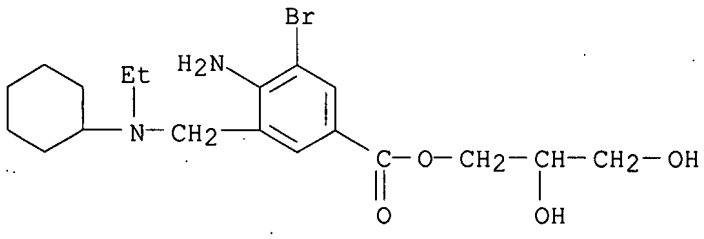
Absolute stereochemistry.



RN 78412-42-7 CAPLUS
CN Benzoic acid, 4-amino-3-bromo-5-[(diethylamino)methyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



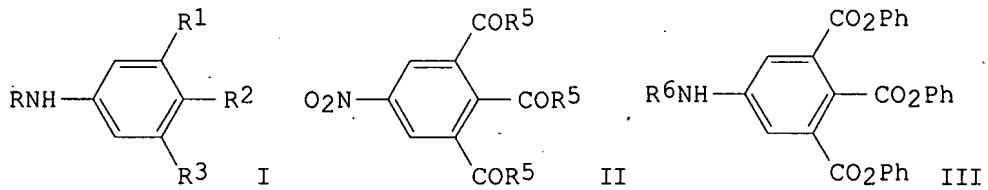
RN 78412-77-8 CAPLUS
CN Benzoic acid, 4-amino-3-bromo-5-[(cyclohexylethylamino)methyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 18 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1981:442668 CAPLUS
DN 95:42668
TI 4-(Monoalkylamino)benzene polycarboxylic acids
IN Shepherd, Robert G.
PA American Cyanamid Co., USA
SO U.S., 8 pp.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4245120	A	19810113	US 1977-836945	19770927
	US 4245119	A	19810113	US 1978-959537	19781113
PRAI	US 1977-836945	A3	19770927		

OS MARPAT 95:42668
GI



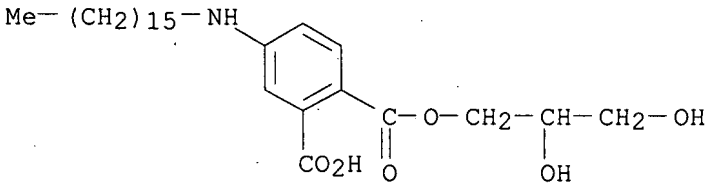
AB Title compds. I [R = C8-19 alkyl; R1, R2, and R3 = H or CO2R4 (R4 = H, C1-4 alkyl, carboxalkyl, hydroxyalkyl dihydroxyalkyl, dialkylaminohydroxyalkyl, polymethyleneiminohydroxyalkyl, Ph, halophenyl, carboxyphenyl, CH2Ph, halobenzyl, carboxybenzyl, pyridylmethyl, halopyridylmethyl, carboxypyridylmethyl, 3-pyridyl, halo-3-pyridyl, carboxy-3-pyridyl, alkali metal cations, alkaline earth metal cations); only one member of R1, R2, or R2 can be H] were prepared as hypolipemics and antiatherosclerotic agents. Thus, 1,2,3-benzenetricarboxylic acid was

nitrated to give nitrobenzene II (R5 = OH), which was treated with SOCl2 to give II (R5 = Cl), which was esterified with PhOH to give II (R5 = OPh). The latter was hydrogenated over Pd/C to give aminobenzenetricarboxylate III (R6 = H), which was alkylated with 1-bromohexadecane to give III (R6 = hexadecyl), which was saponified to give I (R = hexadecyl, R1-R3 = CO2H).

IT 78319-28-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 78319-28-5 CAPLUS

CN 1,2-Benzenedicarboxylic acid, 4-(hexadecylamino)-, 1-(2,3-dihydroxypropyl) ester (9CI) (CA INDEX NAME)



L3 ANSWER 19 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1980:220702 CAPLUS

DN 92:220702

TI X-ray contrast material

IN Felder, Ernst; Pitre, Davide

PA Bracco Industria Chimica S.p.A., Italy

SO Patentschrift (Switz.), 9 pp.
CODEN: SWXXAS

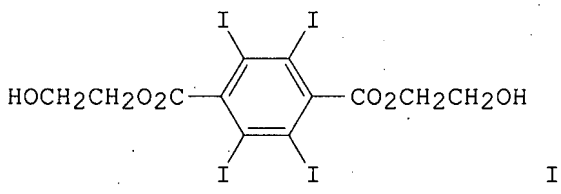
DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	CH 615344	A5	19800131	CH 1975-7800	19750616
PRAI	CH 1975-7800	A	19750616		

GI

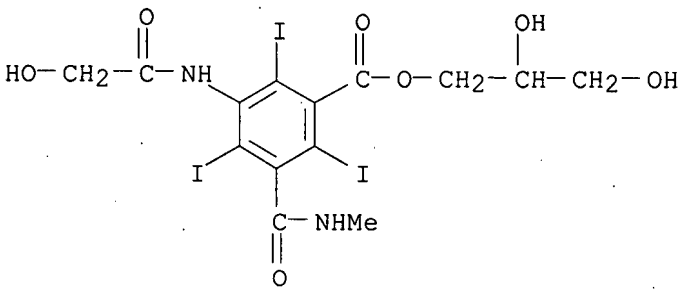


AB An x-ray contrast medium for the lymph system contains a micronized iodobenzoate in a protective colloid. Thus, 358 g micronized I [61838-98-0] was suspended in 370 mL 2% gelatin in 0.9% NaCl, to give a mixture containing 480 mg iodine/mL with a viscosity of 6.1 cP at 37°, pH 7.35, sedimentation quotient of 1 at 2 h and 0.97 at 24 h. The iodobenzoates rapidly cleared from the lymph system and do not cause inflammation. Enlargement of lymph nodes at the injection site is only 10-20%.

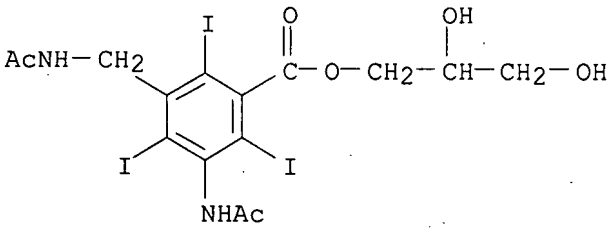
IT 73721-26-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 73721-26-3 CAPLUS

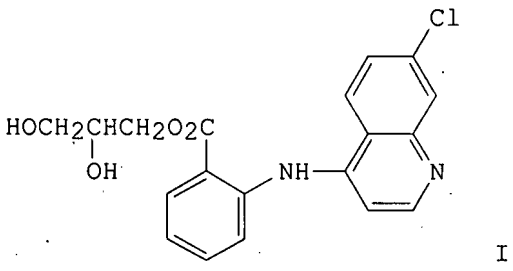
CN Benzoic acid, 3-[(hydroxyacetyl)amino]-2,4,6-triiodo-5-[(methylamino)carbonyl]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



IT 67093-13-4
RL: BIOL (Biological study)
(radiog. contrast media containing)
RN 67093-13-4 CAPLUS
CN Benzoic acid, 3-(acetylamino)-5-[(acetylamino)methyl]-2,4,6-triiodo-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 20 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1980:104420 CAPLUS
DN 92:104420
TI Mechanism of renal effects of large doses of glafenine in the rat
AU Peterfalvi, M.; Deraedt, R.; Pottier, J.; Vannier, B.; Boissier, J. R.
CS Cent. Rech. Roussel-Uclaf, Romainville, 93230, Fr.
SO Therapie (1979), 34(3), 377-91
CODEN: THERAP; ISSN: 0040-5957
DT Journal
LA French
GI



I

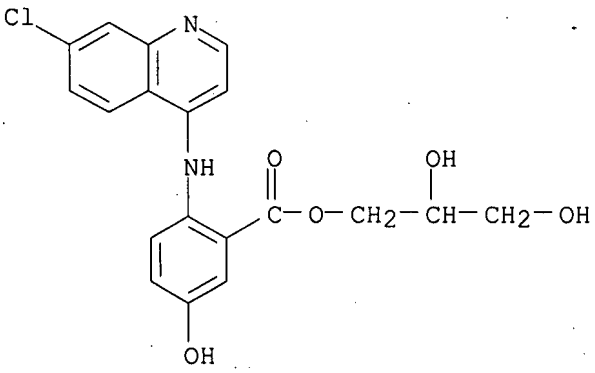
AB In the rat, the oral LD50 of glafenine (I) [3820-67-5] is .apprx.2,300 mg/kg. High oral doses, well above the pharmacol. active ones (2 to 10

mg/kg), induced reversible acute renal failure, the threshold dose being .apprx.200 mg/kg. The kidney damage is characterized by an increase of serum urea, intrarenal water retention and dilation and flattening of the epithelium of the renal tubules. I nephrotoxicity can be avoided by fractionation of the toxic dose in several administrations. The high doses also exerted an antidiuretic effect. The pathogenesis of this acute renal failure is characterized by early obstruction of the collecting tubules by deposits which are yellow colored due to accumulation of the I metabolite, hydroxyglafenic acid [72071-22-8]. Of the urinary metabolites of I only hydroxyglafenic acid was nephrotoxic by i.v. route.

IT 72071-23-9
RL: BIOL (Biological study)
(as glafenine metabolite, toxicity in relation to)

RN 72071-23-9 CAPLUS

CN Benzoic acid, 2-[(7-chloro-4-quinolinyl)amino]-5-hydroxy-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 21 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1980:152 CAPLUS

DN 92:152

TI Biotransformations of glafenine in the rat and in man

AU Pottier, J.; Busigny, M.; Raynaud, J. P.

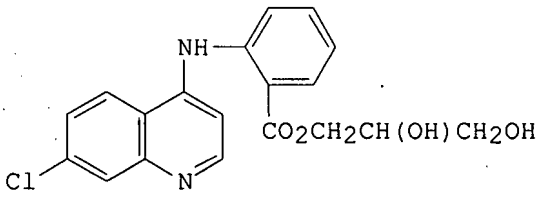
CS Cent. Rech. Roussel-Uclaf, Romainville, 93230, Fr.

SO European Journal of Drug Metabolism and Pharmacokinetics (1979), 4(2), 109-15
CODEN: EJDPD2; ISSN: 0398-7639

DT Journal

LA English

GI



I

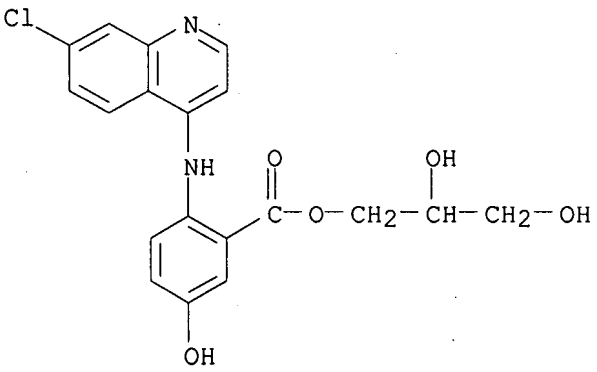
AB The biotransformations of a therapeutic dose of the nonnarcotic analgesic glafenine (I) [3820-67-5], were studied in the rat and in man. In the rat, the ester bond was hydrolyzed to give glafenic acid [10440-42-3] the major metabolite excreted in the bile and urine. Two minor pathways were identified; hydroxylation of the benzene ring of I or glafenic acid para to the amino-substituent and oxidation of the quinoline N of glafenic acid,

to its N-oxide. In vivo, this N-oxide was partly reduced to the parent compound Hydroxyglafenic acid [72071-22-8] was the product of both direct oxidation of glafenic acid and hydrolysis of hydroxyglafenine. The glyceric esters were conjugated as glucuronides and(or) sulfate esters and the carboxylic metabolites as acyl glucuronides. The analogous urinary excretion patterns in man and in the rat suggest a similarity in the biotransformations of I in these 2 species.

IT 72071-23-9
RL: BIOL (Biological study)
(as glafenine metabolite)

RN 72071-23-9 CAPLUS

CN Benzoic acid, 2-[(7-chloro-4-quinolinyl)amino]-5-hydroxy-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 22 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1978:438776 CAPLUS

DN 89:38776

TI Radiopaque contrast media. XLV. Experimental lymphography with crystal suspensions

AU Felder, E.; Pitre, D.; Tirone, P.; Zingales, M. F.

CS Res. Lab., Bracco Ind. Chim. S.p.A., Milan, Italy

SO Farmaco, Edizione Scientifica (1978), 33(4), 302-14
CODEN: FRPSAX; ISSN: 0430-0920

DT Journal

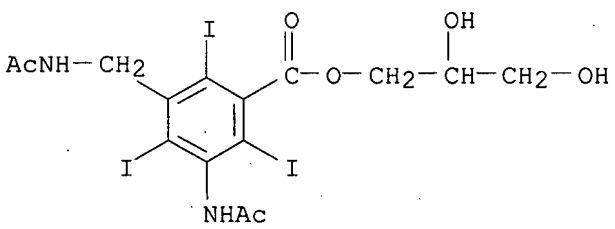
LA English

AB The preparation, properties, toxicity, and pharmacokinetics of iodomide and 2,3,5,6-tetraiodoteraphthalic acid derivs. were presented, and their use in lymphog. was examined in dogs. The iodinated contrast media gave sharp image delineation, and had low viscosity and good miscibility for enhanced lymphatic uptake.

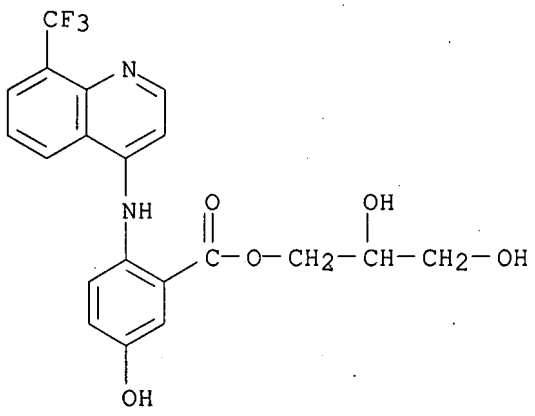
IT 67093-13-4
RL: BIOL (Biological study)
(contrast media, for lymphog.)

RN 67093-13-4 CAPLUS

CN Benzoic acid, 3-(acetylamino)-5-[(acetylamino)methyl]-2,4,6-triiodo-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 23 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1975:471462 CAPLUS
DN 83:71462
TI Pharmacokinetic study of a peripheral analgesic, floctafenin, in man, mouse, rat, and dog
AU Pottier, J.; Busigny, M.; Raynaud, J. P.
CS Cent. Rech., Roussel-Uclaf, Romainville, Fr.
SO Drug Metabolism and Disposition (1975), 3(3), 133-47
CODEN: DMDSAI; ISSN: 0090-9556
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB The pharmacokinetics of floctafenin (I) [23779-99-9] was studied in man, mice, rats, and dogs at pharmacol. doses. Its absorption, which was exclusively intestinal, was good in man and rodents, but only partial in dogs. Its high plasma clearance rate was primarily due to hepatic hydrolysis to floctafenic acid [36783-34-3], which was the main circulating product almost immediately following i.v. administration. This compound bound to 2 sets of binding sites in animal serum and human plasma with affinity consts. of 107M-1 and 105M-1 at 4° in all species except the dog, where binding was weaker. This binding was solely accounted for by albumin. Floctafenin, less protein-bound than floctafenic acid, diffused more widely into tissues, but very low quantities of the ester and virtually negligible quantities of the acid crossed the blood-brain barrier, indicating that their analgesic activity was exclusively peripheral. The elimination of floctafenin and its metabolites was practically complete in 24 hr. The main excretory route was via the bile, biliary excretion being largely predominant in dogs and rats, and somewhat less so in man and mice. There was no enterohepatic cycle of note. The main metabolite in both bile and urine was floctafenic acid. A secondary metabolic pathway, common to all species, led, by hydroxylation in the position para to the anthranilic nitrogen, to the corresponding phenols. All products in man and rats were excreted primarily in the form of ether and/or ester O-glucuronides.
IT 56047-11-1
RL: BIOL (Biological study)
(as floctafenin metabolite, species in relation to)
RN 56047-11-1 CAPLUS
CN Benzoic acid, 5-hydroxy-2-[[8-(trifluoromethyl)-4-quinolinyl]amino]-, 2,3-dihydroxypropyl ester (9CI) (CA INDEX NAME)

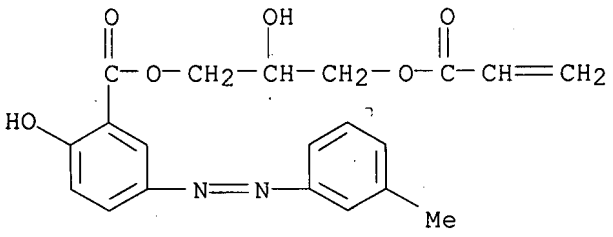


L3 ANSWER 24 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1965:499399 CAPLUS
DN 63:99399

OREF 63:18367f-g
TI Purity of terephthalic acid for conversion into poly(ethylene terephthalate)
PA Toyo Rayon Co., Ltd.
SO 4 pp.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 1000045		19650804	GB 1962-12800	19620403
PRAI	JP		19610417		

AB The purity of terephthalic acid (I) to be esterified directly with ethylene glycol can be tested by a light transmittance method. Thus, the light transmittance of 7.5 g. I in 50 ml. 2N KOH is compared with the transmittance of a 2N KOH standard solution Transmittance measurements are made with a spectrophotometer using a light of 340 mμ wave length and a cell length of 10 mm. Samples with 93-7% transmittances give pure white, polyester fibers. Cf. following abstract
IT 3766-51-6
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 3766-51-6 CAPLUS
CN Salicylic acid, 5-(m-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA INDEX NAME)

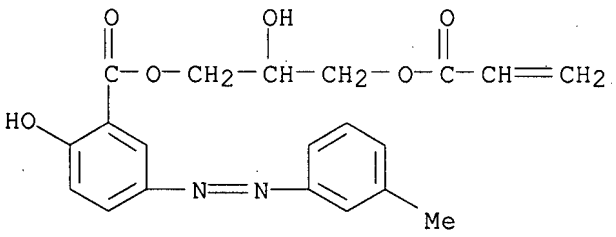


L3 ANSWER 25 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1965:499398 CAPLUS
DN 63:99398
OREF 63:18367e-f
TI Azobenzene-containing polymeric compositions capable of being integrally colored and resistant to ultraviolet light
IN Fertig, Joseph; Goldberg, Albert I.; Skoultchi, Martin
PA National Starch and Chemical Corp.
SO 6 pp.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3190861		19650622	US 1962-205218	19620626
PRAI	US		19620626		

AB Similar to U.S. 3,190,860 (CA 63, 13529c) except that a wide variety of copolymers derived from novel azobenzene monomers are effectively stabilized against uv radiation without requiring the addition of extraneous uv absorbers to the polymer. The use of these novel monomers in higher concns. results in the preparation of copolymers which, in addition to their enhanced light stability, also have an unextractable "built in" color. The color is determined by selection of the proper azobenzene compound
IT 3766-51-6
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 3766-51-6 CAPLUS
CN Salicylic acid, 5-(m-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA

INDEX NAME)



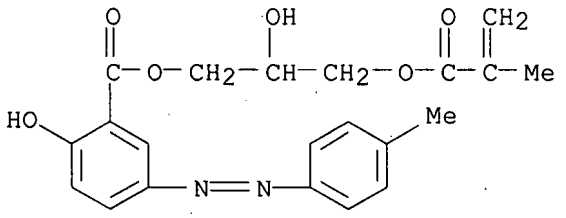
L3 ANSWER 26 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1965:480362 CAPLUS
DN 63:80362
OREF 63:14761b-e
TI Ethylenically unsaturated derivatives of azobenzene
IN Skoultchi, Martin M.; Goldberg, Albert I.; Joseph Fertig
PA National Starch and Chemical Corp.
SO 5 pp.
DT Patent
LA Unavailable
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3190874		19650622	US 1962-188861	19620419
	GB 1006884			GB	
PRAI	US		19620419		

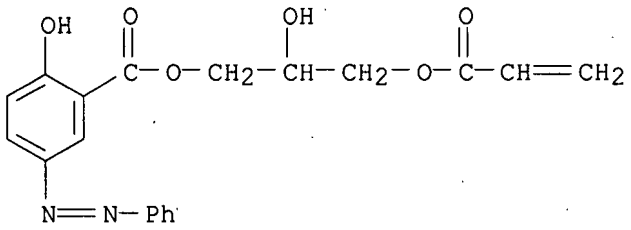
AB The title compds. were prepared by treating glycidyl acrylate or the methacrylate (I) with a carboxylated azobenzene in the presence of a catalyst. Thus, to a stirred mixture of I 156 and 50% aqueous NaOH 3.2, 5-phenylazo-2-hydroxybenzoic acid (II) 242 parts was added during 1 hr. at 70-80° the mixture stirred 7 hrs. at 70-80°, and cooled to room temperature to give 94% CH2:CRCO2CH2CH(OH)CH2R1 (III) (R = Me, R1 = 5-phenylazo-2-hydroxybenzoyloxy), tan in color but yellow-orange in organic solvents. Similarly prepared were III (R = Me) (R1and % yield given): 4-phenylazobenzoyloxy, 93; 2-phenylazobenzoyloxy, 80; 4-(4-methylphenylazo)benzoyloxy, 92; 5-(4-methylphenylazo)-2-hydroxybenzoyloxy, 94.5; 5-(3-methylphenylazo)-2-hydroxybenzoyloxy, 95; 5-(2-methylphenylazo)-2-hydroxybenzoyloxy, 95; 4-(2-chlorophenylazo)benzoyl oxy, 85; 4-(2-methoxyphenylazo)benzoyloxy, 86; 4-(4-phenylphenylazo)benzoyloxy, 83; 4-(2-naphthylazo)benzoyloxy, 93; and III (R = H) (R1 and % yield given): 4-phenylazobenzoyloxy, 94; 2-phenylazobenzoyloxy, 83; 4-(4-methylphenylazo)benzoyloxy, 92.5; 5-(4-methylphenylazo)-2-hydroxybenzoyloxy, 95; 5-(3-methylphenylazo)-2-hydroxybenzoyloxy, 95; 5-(2-methylphenylazo)-2-hydroxybenzoyloxy, 95; 4-(2-chlorophenylazo)benzoyloxy, 89; 4-(2-methoxyphenylazo)benzoyloxy, 83; 4-(4phenylphenylazo)benzoyloxy, 75; 4-(2-naphthylazo)benzoyloxy, 92. Cf. following 2 abstrs.

IT 3758-48-3P, Salicylic acid, 5-(p-tolylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate 3766-36-7P, Salicylic acid, 5-(phenylazo)-, 2,3-dihydroxypropyl ester, 3-acrylate 3766-39-0P , Salicylic acid, 5-(phenylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate 3766-42-5P, Salicylic acid, 5-(m-tolylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate 3766-43-6P, Salicylic acid, 5-(o-tolylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate 3766-50-5P, Salicylic acid, 5-(p-tolylazo)-, 2,3-dihydroxypropyl ester, 3-acrylate 3766-51-6P, Salicylic acid, 5-(m-tolylazo)-, 2,3-dihydroxypropyl ester, 3-acrylate 3766-52-7P, Salicylic acid, 5-(o-tolylazo)-, 2,3-dihydroxypropyl ester, 3-acrylate
RL: PREP (Preparation)
(preparation of)

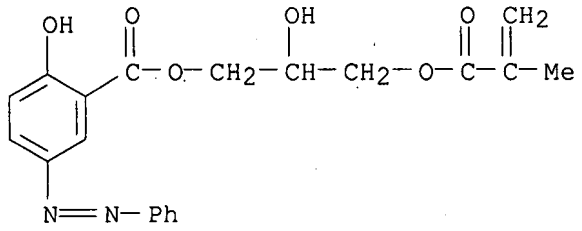
RN 3758-48-3 CAPLUS
CN Salicylic acid, 5-(p-tolylazo)-, 2,3-dihydroxypropyl ester, 3-methacrylate (7CI, 8CI) (CA INDEX NAME)



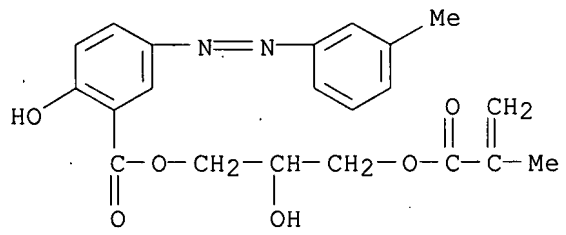
RN 3766-36-7 CAPLUS
CN Salicylic acid, 5-(phenylazo)-, 3-ester with 1-monoacrylin (8CI) (CA INDEX NAME)



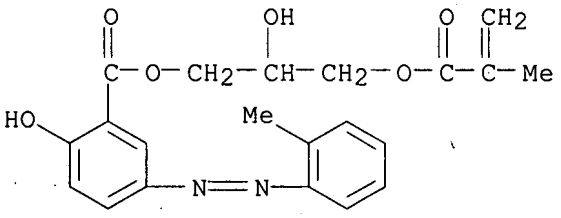
RN 3766-39-0 CAPLUS
CN Salicylic acid, 5-(phenylazo)-, 2,3-dihydroxypropyl ester 3-methacrylate (7CI, 8CI) (CA INDEX NAME)



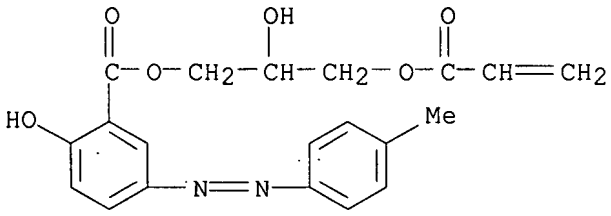
RN 3766-42-5 CAPLUS
CN Salicylic acid, 5-(m-tolylazo)-, 2,3-dihydroxypropyl ester 3-methacrylate (7CI, 8CI) (CA INDEX NAME)



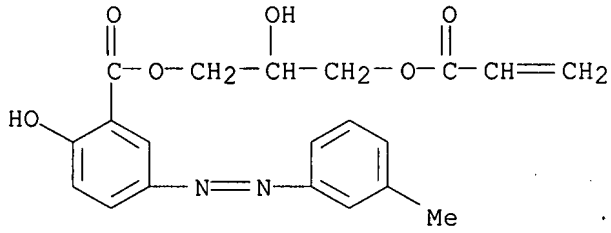
RN 3766-43-6 CAPLUS
CN Salicylic acid, 5-(o-tolylazo)-, 2,3-dihydroxypropyl ester 3-methacrylate (7CI, 8CI) (CA INDEX NAME)



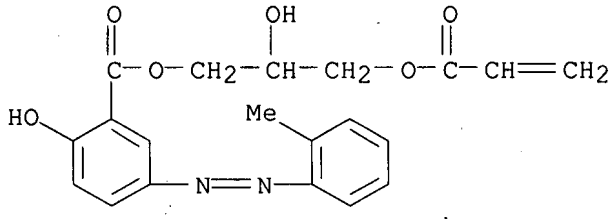
RN 3766-50-5 CAPLUS
CN Salicylic acid, 5-(p-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA INDEX NAME)



RN 3766-51-6 CAPLUS
CN Salicylic acid, 5-(m-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA INDEX NAME)



RN 3766-52-7 CAPLUS
CN Salicylic acid, 5-(o-tolylazo)-, 3-ester with 1-monoacrylin (8CI) (CA INDEX NAME)

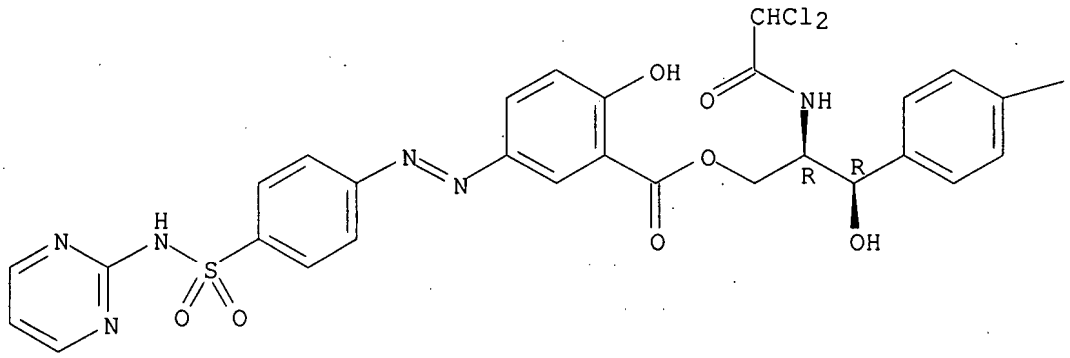


L3 ANSWER 27 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1965:2810 CAPLUS
DN 62:2810
OREF 62:464e-g
TI Synthesis of chloramphenicol derivatives and their preliminary microbiological assay
AU Jaramillo, M. V. H.; v. Plessing B., Carlos

SO Farm. Nueva (Madrid) (1964), 29(329), 253-62
DT Journal
LA Spanish
GI For diagram(s), see printed CA Issue.
AB Dropwise addition of 2.2 g. salicyl chloride to a stirred cooled solution of 2.3
g. chloramphenicol in 5 ml. dioxane containing 0.5 g. NaHCO3, the mixture kept 3
hrs. at room temperature, 100 ml. H2O containing 0.3 ml. HCl added, and the precipitate
collected after 2 hrs. and recrystd. from 15:3 EtOH-H2O at 60° gave 1.522 g. white crysts. chloramphenicol (I) salicylate, m. 144-6°, [α]18D, 40.5° (absolute alc.) (ir and uv spectra given). Sulfadiazine (3.8 g.) in 12 ml. water acidified with 4.5 ml. concentrated HCl was diazotized at 4° by addition of 4.3 ml. 25% NaNO2 and the product added to an ice-cold solution of 6.6 g. I in 28 ml. 9% NaOH (pH 8.0-8.5); after stirring 30 min., the solution was acidified to precipitate 94.7% 5-[p-(2-pyrimidylsulfamoyl)-phenylazo]salicylate (II) of I, m. 142-3° (alc.), (α)18D 71.5° (absolute alc.) (ir and uv spectra given). Results of pharmacol. tests were given.
IT 6868-03-7P, Salicylic acid, 5-[[p-(2-pyrimidinylsulfamoyl)phenyl]azo]-, α-ester with 2,2-dichloro-N-[β-hydroxy-α-(hydroxymethyl)-p-nitrophenethyl]acetamide
RL: PREP (Preparation)
(preparation and bactericidal action of)
RN 6868-03-7 CAPLUS
CN Salicylic acid, 5-[[p-(2-pyrimidinylsulfamoyl)phenyl]azo]-, α-ester with 2,2-dichloro-N-[β-hydroxy-α-(hydroxymethyl)-p-nitrophenethyl]acetamide (7CI, 8CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

PAGE 1-A

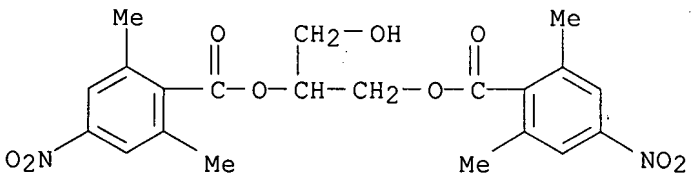


PAGE 1-B

—NO2

L3 ANSWER 28 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1962:436109 CAPLUS
DN 57:36109
OREF 57:7162h-i
TI Chemistry of lactones. VI. Reaction of unsaturated azlactones under Friedel-Crafts conditions

AU Filler, Robert; Rao, Y. Shyamsunder
CS Illinois Inst. of Technol., Chicago
SO Journal of Organic Chemistry (1962), 27, 2403-6
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA Unavailable
AB cf. CA 55, 25906b. The behavior of unsatd. azlactones under Friedel-Crafts conditions has been studied in detail. The course of the reaction is dependent on a variety of factors, including reaction conditions, solvent, and the nature of substituents on the arylidene ring. Four different products have been isolated: saturated azlactones, w-benzamidoacetophenone, 2-benzamidoindenone, and 1-phenylisoquinoline-3-carboxylic acids.
IT 94862-60-9P, Benzoic acid, 2,6-dimethyl-4-nitro-, (hydroxymethyl)ethylene ester
RL: PREP (Preparation)
(preparation of)
RN 94862-60-9 CAPLUS
CN Benzoic acid, 2,6-dimethyl-4-nitro-, (hydroxymethyl)ethylene ester (7CI) (CA INDEX NAME)

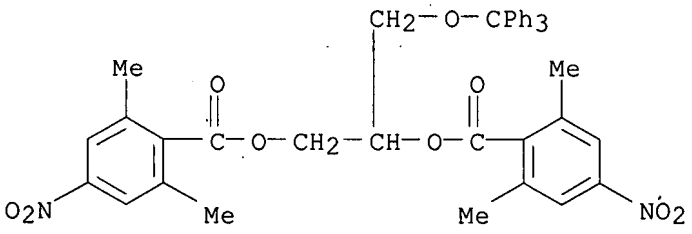


L3 ANSWER 29 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1962:436108 CAPLUS
DN 57:36108
OREF 57:7162c-h
TI Migration of an acyl group in glycerol derivatives. II. Transformation of diacylglycerol-β-iodohydrins into diphenyl diacylglycerol-a-phosphates
AU Hoefnagel, M. A.; Hartman-Kohler, A. H.; Verkade, P. E.
CS Tech. Univ., Delft, Neth.
SO Recueil des Travaux Chimiques des Pays-Bas (1961), 80, 608-22
CODEN: RTCPA3; ISSN: 0165-0513
DT Journal
LA Unavailable
AB cf. CA 54, 22387h. 2,6,4-Me2(O2N)C6H2CO2H and SOCl2 (1:3) refluxed 3 hrs. gave 93% 2,6,4-Me2(O2N)C6H2COCl (I), b21 168.5-9°, m. 60.5-1.5°. To 6.73 g. HOCH2 CHICH2OH (II), 30 ml. dry CHCl3, and 6 ml. dry C5H5N was added 20.3 g. C17H35COCl in 30 ml. dry CHCl3 and the whole kept 4 days in the dark at 30-5° to give 28.8 g. C17H35CO2CH2CHICH2O2CC17H35 (IIa), m. 57-8° (petr. etherabs. MeOH). To 8.08 g. HOCH2CH(OH)CH2 (III), 40 ml. dry C6H6, and 12 ml. pure Et3N was added 13.92 g. p-MeOC6H4COCl (IIIa), and the whole kept 6 days in the dark at room temperature gave 16.72 g. p-MeOC6H4CO2CH2CH (O2CC6H4OMe-p)CH2 (IV), m. 94-5° (C6H6-petr. ether); II similarly gave 98% p-MeOC6H4CO2CH2CHICH2O2CC6H4OMe-p (V), m. 69-70° (EtOAc-MeOH); II and I gave 93% 2,6,4-Me2(O2N)C6H2CO2CHICH2O2CC6(O2N)Me2-4,6,2 (VI), m. 154-5° (C6H6-MeOH); I and III gave a poor yield of 2,6,4-Me2(O2N)C6H2CO2CH2CH[O2CC6H2(O2N)Me2 4,6,2]CH2I (VII), m. 174.5-5.5° (EtOAcMeOH). IIa (2.49 g.), 60 ml. C6H6, and 1.57 g. (PhO)2-PO(OAg) (VIII) refluxed 6 hrs. gave 3.22 g. α-phosphate derivative, m. 58-9° (petr. ether); in similar fashion, IV and VIII gave 94% of α-phosphate (IX), m. 64-6.5° (Et2Opetr. ether); V and VIII also gave IX; both VI and VII with VIII gave the

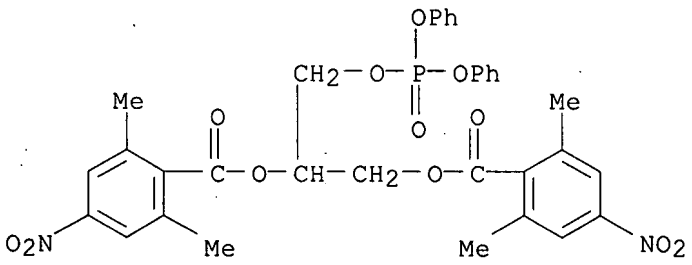
α-phosphate (X), m. 112-13° (MeOH). To Ph3COCH2CH(OH)CH2OH (XI) in 15 ml. dry C5H5N was added 6.0 g. IIIa and the whole kept several days at room temperature gave 92% Ph3COCH2CH(O2CC6H4OMe-p)CH2O2CC6H4OMe-p (XII), m. 134.5-5° (EtOAc-petr. ether); alternately, 2.55 g. p-MeOC6H4CO2CH2CH(O2CC6H4OMe-p)CH2OH (XIII), 2.42 g. Ph3CBr (XIV) and 35 ml. dry C5H5N kept 8 hrs. at 100° gave 3.49 g. XII. XI (1.67 g.), 2.3 g. I, and 30 ml. pure Et3N kept 12 days at room temperature gave 1.50 g. Ph3COCH2CH[O2CC6H2(O2N)Me2-4,6,2]CH2O2CC6H2(O2N)Me2-4,6,2 (XV), m. 172-3°; alternately, XIV and 2,6,4-Me2(O2N)C6H2CO2CH[O2CC6H2(NO2)Me 2-4,6,2]CH2OH, as above, also gave XV. XII (12.04 g.), 200 ml. absolute EtOH, and Pd-C (from 1 g. PdCl2) shaken 5 hrs. at 65-75° with H, the whole filtered, the EtOH distilled and the residue dissolved in 180 ml. petr. ether gave 6.73 g. p-MeOC6H4CO2CH2CH(O2CC6H4OMe-p)CH2OH, m. 62.5-3.5°. At 0°, to 2.05 g. XV in 3 ml. C6H6 and 5 ml. glacial AcOH was added 6 ml. HBr saturated AcOH, the whole kept 5 min. at 0° the XIV filtered, the filtrate in 125 ml. Et2O washed with H2O, 5% KHCO3, dried, and concentrated gave 1.13 g. 2,6,4-Me2(O2N)C6H2CO2CH2CH [O2CC6H2(NO2)Me24,6,2]CH2OH, m. 138-9° (C6H6-MeOH).

IT 96871-82-8P, Benzoic acid, 2,6-dimethyl-4-nitro-, [(trityloxy)methyl]ethylene ester 97658-12-3P, Benzoic acid, 2,6-dimethyl-4-nitro-, (hydroxymethyl)ethylene ester, di-Ph phosphate
RL: PREP (Preparation)
(preparation of)

RN 96871-82-8 CAPLUS
CN Benzoic acid, 2,6-dimethyl-4-nitro-, [(trityloxy)methyl]ethylene ester (7CI) (CA INDEX NAME)

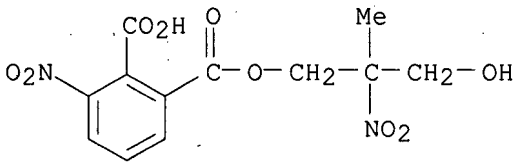


RN 97658-12-3 CAPLUS
CN Benzoic acid, 2,6-dimethyl-4-nitro-, (hydroxymethyl)ethylene ester, diphenyl phosphate (7CI) (CA INDEX NAME)



L3 ANSWER 30 OF 30 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1954:25061 CAPLUS
DN 48:25061
OREF 48:4548b-d
TI Less known properties of nitro compounds
AU Urbanski, Tadeusz
CS Inst. Technol., Warsaw
SO Roczniki Chemii (1951), 25, 257-84;English summary, 284-6

CODEN: ROCHAC; ISSN: 0035-7677
DT Journal
LA Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 46, 7993c. A review of chemical properties of nitro compds. is presented. Unpublished so far, the preparation of a number of pyrimidine compds.
of the type (I) from MeNO2 is mentioned; also a tetrahydrooxazine compound (II) was obtained from PhCH2NO2.
IT 856806-60-5P, Phthalic acid, 3-nitro-, ester with 2-methyl-2-nitro-1,3-propanediol
RL: PREP (Preparation)
(preparation of)
RN 856806-60-5 CAPLUS
CN Phthalic acid, 3-nitro-, ester with 2-methyl-2-nitro-1,3-propanediol (5CI) (CA INDEX NAME)



JC 6/20/07

STN SSS search

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

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NEWS 3	MAR 16	CASREACT coverage extended
NEWS 4	MAR 20	MARPAT now updated daily
NEWS 5	MAR 22	LWPI reloaded
NEWS 6	MAR 30	RDISCLOSURE reloaded with enhancements
NEWS 7	APR 02	JICST-EPLUS removed from database clusters and STN
NEWS 8	APR 30	GENBANK reloaded and enhanced with Genome Project ID field
NEWS 9	APR 30	CHEMCATS enhanced with 1.2 million new records
NEWS 10	APR 30	CA/CAplus enhanced with 1870-1889 U.S. patent records
NEWS 11	APR 30	INPADOC replaced by INPADOCDB on STN
NEWS 12	MAY 01	New CAS web site launched
NEWS 13	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 14	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 15	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 16	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 17	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 18	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 19	JUN 18	CA/CAplus to be enhanced with pre-1967 CAS Registry Numbers

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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NEWS IPC8	For general information regarding STN implementation of IPC 8

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FILE 'HOME' ENTERED AT 09:54:02 ON 20 JUN 2007

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.42	0.42

FILE 'REGISTRY' ENTERED AT 09:55:03 ON 20 JUN 2007
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STRUCTURE FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1
DICTIONARY FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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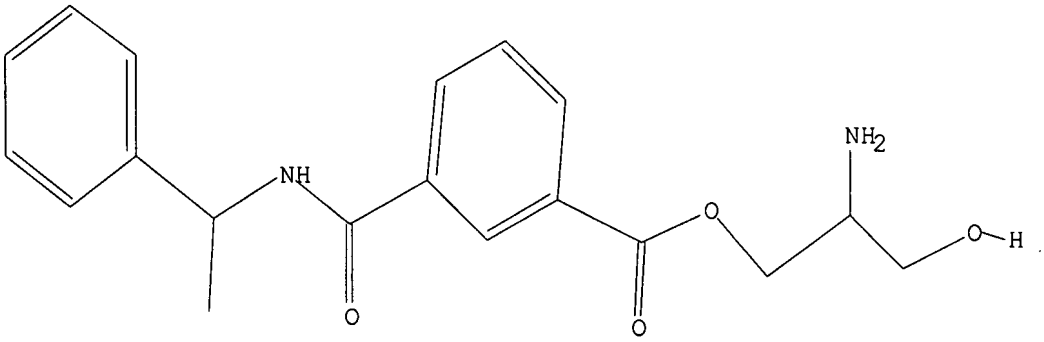
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 6 TO ITERATE

100.0% PROCESSED 6 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
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PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full
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FULL SCREEN SEARCH COMPLETED - 116 TO ITERATE

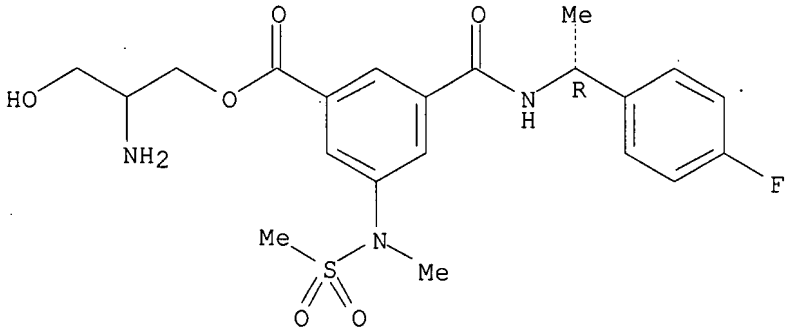
100.0% PROCESSED 116 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

L3 5 SEA SSS FUL L1

=> d scan

L3 5 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-3-hydroxypropyl ester (9CI)
MF C21 H26 F N3 O6 S

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 172.55 172.97

FILE 'CAPLUS' ENTERED AT 09:56:23 ON 20 JUN 2007
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FILE COVERS 1907 - 20 Jun 2007 VOL 146 ISS 26

FILE LAST UPDATED: 19 Jun 2007 (20070619/ED)

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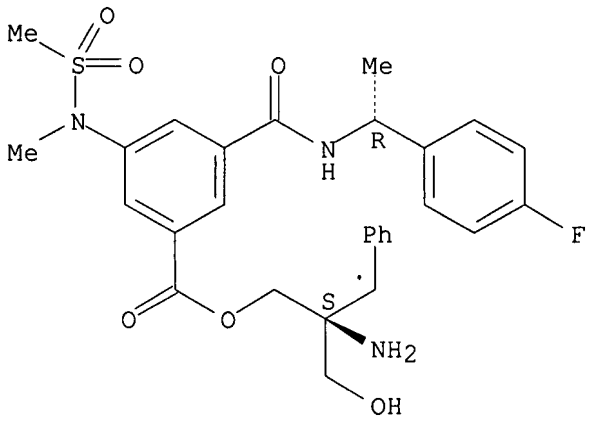
http://www.cas.org/infopolicy.html

=> s l3
L4 2 L3

=> d l4 1-2 bib abs hitstr

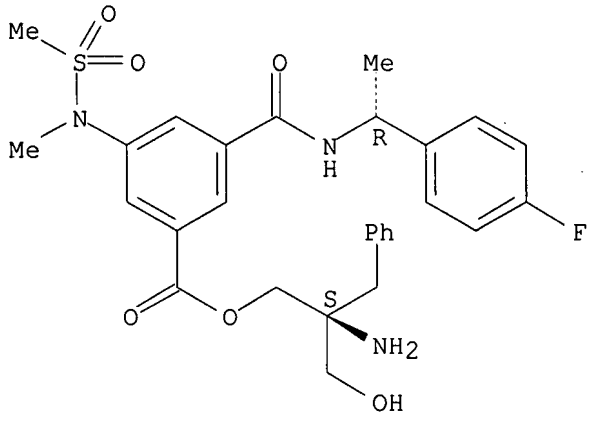
L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1191598 CAPLUS
DN 146:116781
TI Discovery of Oxadiazoyl Tertiary Carbinamine Inhibitors of β-Secretase (BACE-1)
AU Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick, Harold G.; Munshi, Sanjeev; McGaughey, Georgia B.; Lindsley, Stacey R.; Young, Mary Beth; Lai, Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi, Dennis; Pietrak, Beth; Crouthamel, Ming-Chih; Tugusheva, Katherine; Huang, Qian; Xu, Min; Simon, Adam J.; Kuo, Lawrence; Hazuda, Daria J.; Graham, Samuel; Vacca, Joseph P.
CS Departments of Medicinal Chemistry, Structural Biology, Molecular Systems and Alzheimer's Research, Merck Research Laboratories, West Point, PA, 19486, USA
SO Journal of Medicinal Chemistry (2006), 49(25), 7270-7273
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
OS CASREACT 146:116781
AB We describe the discovery and optimization of tertiary carbinamine derived inhibitors of the enzyme β-secretase (BACE-1). These novel non-transition-state-derived ligands incorporate a single primary amine to interact with the catalytic aspartates of the target enzyme. Optimization of this series provided inhibitors with intrinsic and functional potency comparable to evolved transition state isostere derived inhibitors of BACE-1.
IT 918344-77-1 918344-77-1D, complexes with β-secretase
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(discovery of oxadiazoyl tertiary carbinamine inhibitors of β-secretase)
RN 918344-77-1 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



RN 918344-77-1 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, (2S)-2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:55021 CAPLUS
DN 142:134323
TI Preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease
IN Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005004803	A2	20050120	WO 2004-US20525	20040625
	WO 2005004803	A3	20050421		

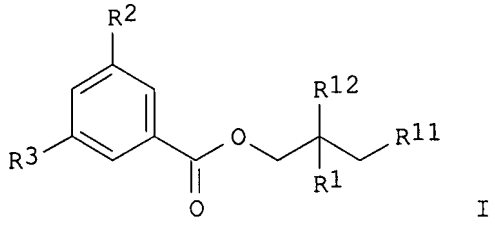
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,

NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004255191	A1	20050120	AU 2004-255191	20040625
CA 2530006	A1	20050120	CA 2004-2530006	20040625
EP 1643986	A2	20060412	EP 2004-756168	20040625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1909897	A	20070207	CN 2004-80018651	20040625
US 2006149092	A1	20060706	US 2005-562470	20051222
PRAI US 2003-484150P	P	20030701		
WO 2004-US20525	W	20040625		

OS MARPAT 142:134323

GI



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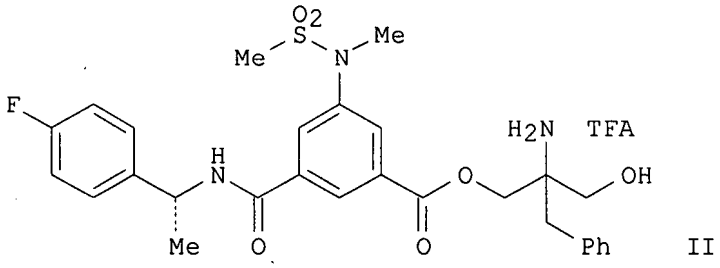


II

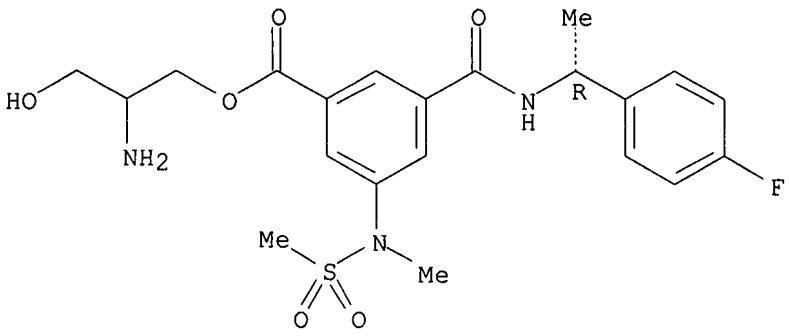
AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl, alkenyl, alkynyl, Ph, PhCH2; R7 = H, alkyl, alkenyl, alkynyl; R3 = (substituted) PhCHR5NHCO, R9R10NHCO, etc.; R9R10 = atoms to form (substituted) pyrrolidinyl, piperidinyl; R11 = OH, alkoxy, phenylalkoxy, PhO, Ph; R12 = NR9R10, OH], were prepared as β-secretase inhibitors for the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

IT 827039-53-2P 827039-54-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)

RN 827039-53-2 CAPLUS

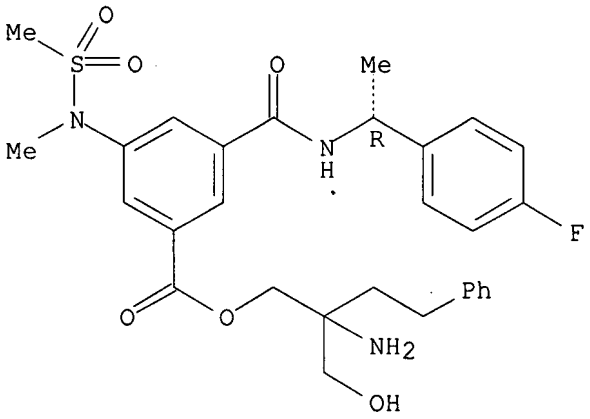
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-3-hydroxypropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 827039-54-3 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-4-phenylbutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

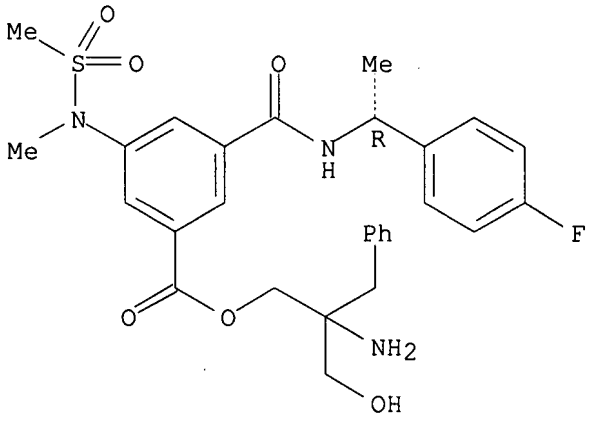


IT 827039-74-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)
RN 827039-74-7 CAPLUS
CN Benzoic acid, 3-[[[(1R)-1-(4-fluorophenyl)ethyl]amino]carbonyl]-5-[methyl(methylsulfonyl)amino]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

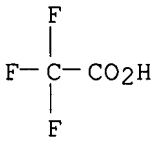
CRN 827039-73-6
CMF C28 H32 F N3 O6 S

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	11.48	184.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.56	-1.56

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STRUCTURE FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1
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http://www.cas.org/support/stngen/stndoc/properties.html

=>
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L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l5 sss sam
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SAMPLE SCREEN SEARCH COMPLETED - 1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1 TO 80
PROJECTED ANSWERS: 1 TO 80

L6 1 SEA SSS SAM L5

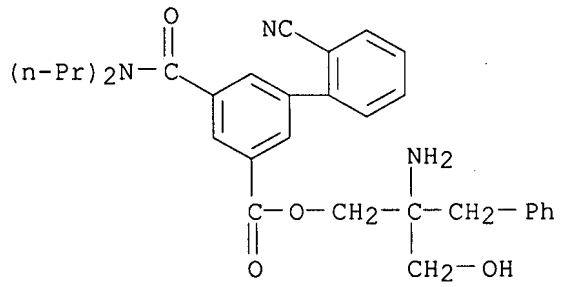
=> s l5 sss full
FULL SEARCH INITIATED 09:58:56 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L7 2 SEA SSS FUL L5

=> d scan

L7 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[(dipropylamino)carbonyl]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI)
MF C31 H35 N3 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus
COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION
FULL ESTIMATED COST | 173.00 | 357.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION
CA SUBSCRIBER PRICE | 0.00 | -1.56

FILE 'CAPLUS' ENTERED AT 09:59:09 ON 20 JUN 2007
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FILE COVERS 1907 - 20 Jun 2007 VOL 146 ISS 26
FILE LAST UPDATED: 19 Jun 2007 (20070619/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l7
L8 1 L7

=> d l8 bib abs hitstr

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:55021 CAPLUS
DN 142:134323
TI Preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease
IN Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005004803	A2	20050120	WO 2004-US20525	20040625
	WO 2005004803	A3	20050421		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,

EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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OS MARPAT 142:134323

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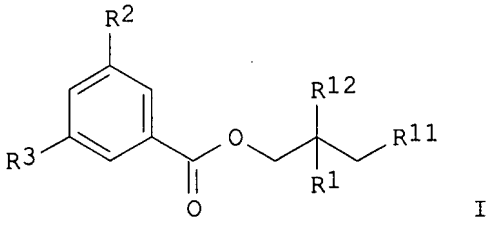

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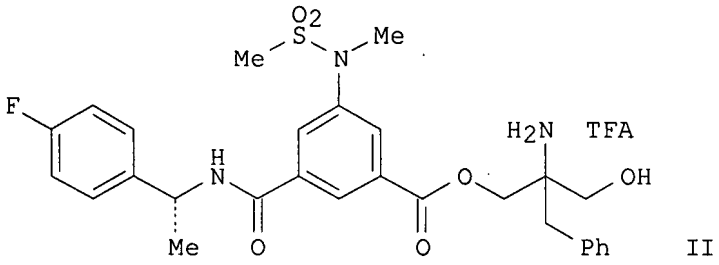


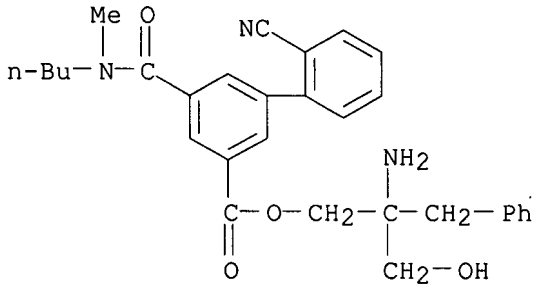
II

AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl, alkenyl, alkynyl, Ph, PhCH2; R7 = H, alkyl, alkenyl, alkynyl; R3 = (substituted) PhCHR5NHCO, R9R10NHCO, etc.; R9R10 = atoms to form (substituted) pyrrolidinyl, piperidinyl; R11 = OH, alkoxy, phenylalkoxy, PhO, Ph; R12 = NR9R10, OH], were prepared as β-secretase inhibitors for the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

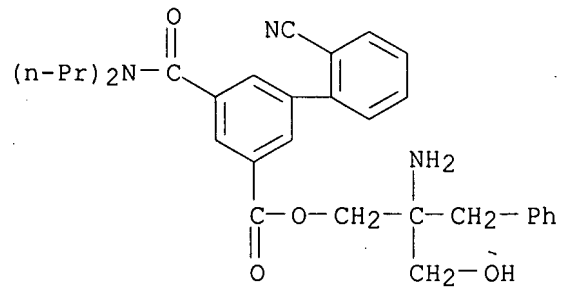
IT 827039-57-6P 827039-62-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)

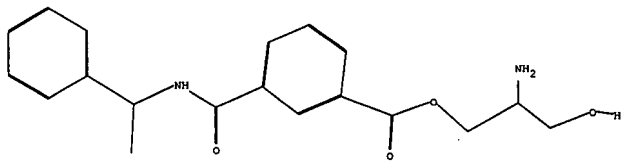
RN 827039-57-6 CAPLUS

CN [1,1'-Biphenyl]-3-carboxylic acid, 5-[(butylmethylamino)carbonyl]-2'-cyano-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)



RN 827039-62-3 CAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[(dipropylamino)carbonyl]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)

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O
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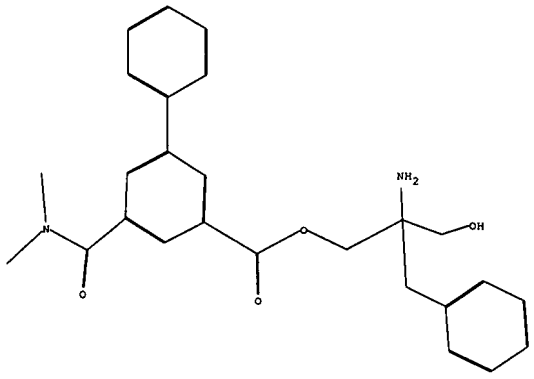
O
H


NH2
OH
N
O
O
O

JC 6/20/07
STN SSS Search.

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJYC1621

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 10:32:39 ON 20 JUN 2007
FILE 'REGISTRY' ENTERED AT 10:32:39 ON 20 JUN 2007

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.90	1.11

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.90	1.11

FILE 'REGISTRY' ENTERED AT 10:32:52 ON 20 JUN 2007

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1
DICTIONARY FILE UPDATES: 19 JUN 2007 HIGHEST RN 937844-74-1

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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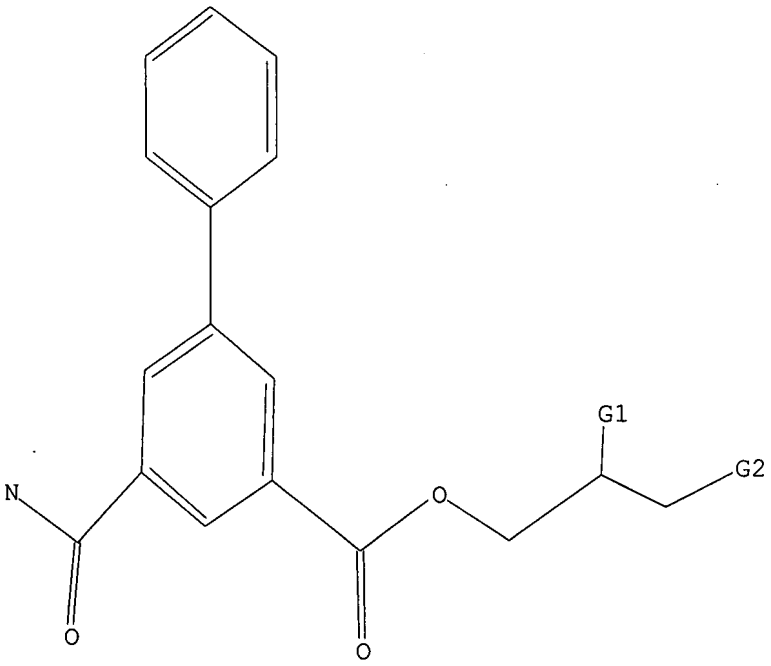
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
SEARCH FAILED DUE TO A STRUCTURE QUERY ERROR
The structure query could not be searched. Please review and revise your structure query, especially checking the variable definitions and attachments. In rare instances the failure may be due to a system problem. Please contact your local STN Help Desk if you need assistance.

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Uploading C:\Documents and Settings\jcho2\My Documents\10562470-f.str

L3 STRUCTURE UPLOADED

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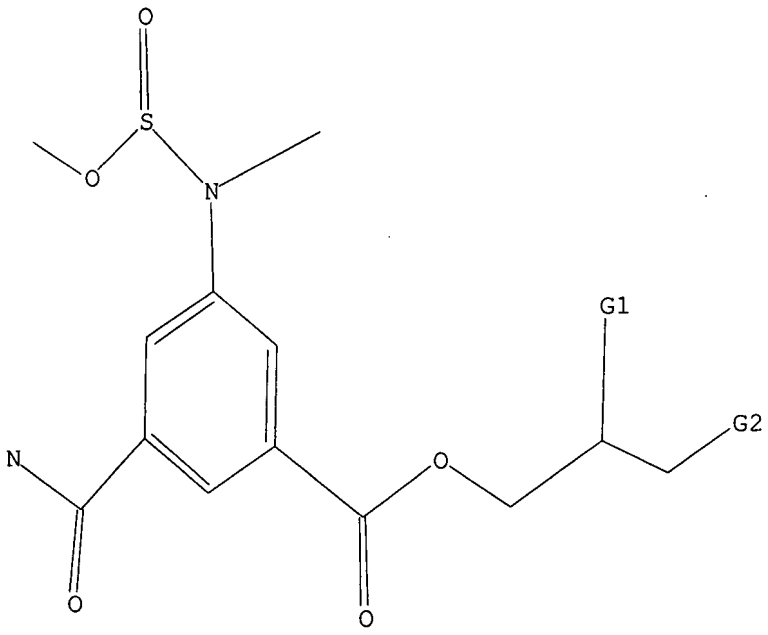
L3 HAS NO ANSWERS
L3 STR



G1 O,N

G2 Ph,O

Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED -        0 TO ITERATE

100.0% PROCESSED        0 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.01

L4            0 SEA SSS FUL L3

=>
Uploading C:\Documents and Settings\jcho2\My Documents\10562470-g.str

L5      STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5              STR
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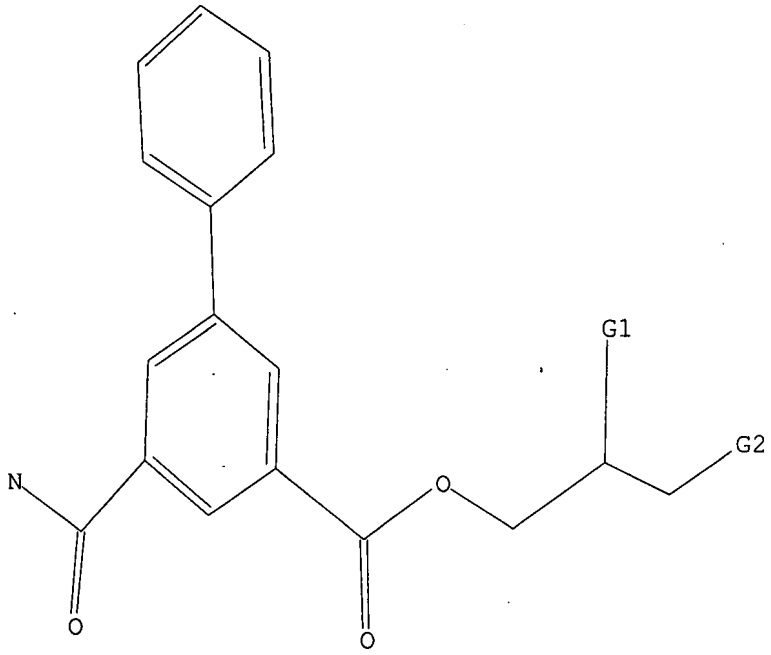


G1 O,N

G2 Ph,O

Structure attributes must be viewed using STN Express query preparation.

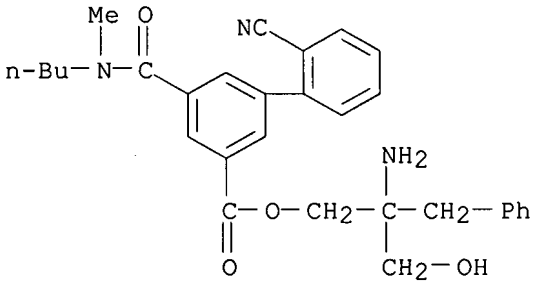
=> s l5 sss full
FULL SEARCH INITIATED 10:35:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 23 TO ITERATE

100.0% PROCESSED 23 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

L6 2 SEA SSS FUL L5

=> d scan

L6 2 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN [1,1'-Biphenyl]-3-carboxylic acid, 5-[(butylmethylamino)carbonyl]-2'-cyano-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI)
MF C30 H33 N3 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   346.00     347.11

FILE 'CAPLUS' ENTERED AT 10:36:14 ON 20 JUN 2007
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FILE COVERS 1907 - 20 Jun 2007  VOL 146 ISS 26
FILE LAST UPDATED: 19 Jun 2007  (20070619/ED)

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http://www.cas.org/infopolicy.html

=> s l2
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




SAMPLE SEARCH INITIATED 10:36:21 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -        2 TO ITERATE

100.0% PROCESSED        2 ITERATIONS                              1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:            2 TO      124
PROJECTED ANSWERS:               1 TO       80

L7            1 SEA SSS SAM L2



L8          1 L7

=> s l6
L9          1 L6

=> d l9 bib abs hitstr

L9   ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2007 ACS on STN
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AN 2005:55021 CAPLUS
DN 142:134323
TI Preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease
IN Nantermet, Philippe G.; Rajapakse, Hemaka Anthony; Selnick, Harold G.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005004803	A2	20050120	WO 2004-US20525	20040625
	WO 2005004803	A3	20050421		
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	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	CA 2530006	A1	20050120	CA 2004-2530006	20040625
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OS MARPAT 142:134323
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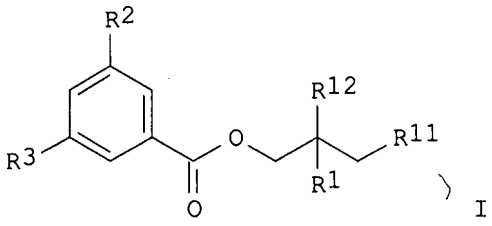

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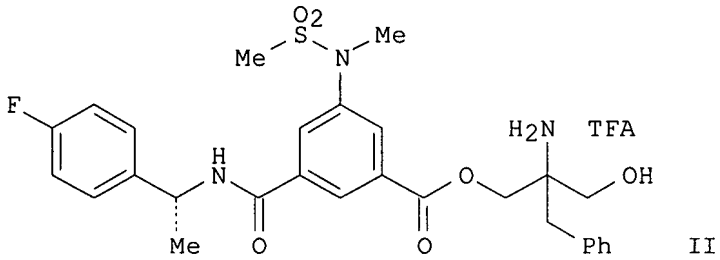


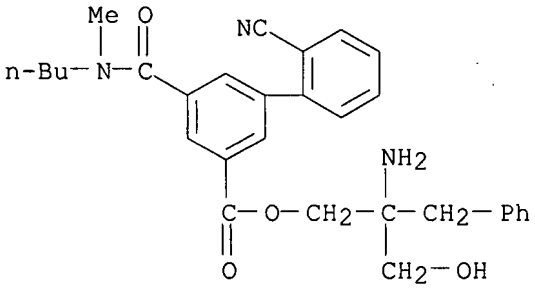
II

AB Title compds. [I; R1, R5, R9, R10 = H, (substituted) alkyl, alkenyl, alkynyl; R2 = R4SO2NR7, (substituted) Ph; R4 = (substituted) alkyl,

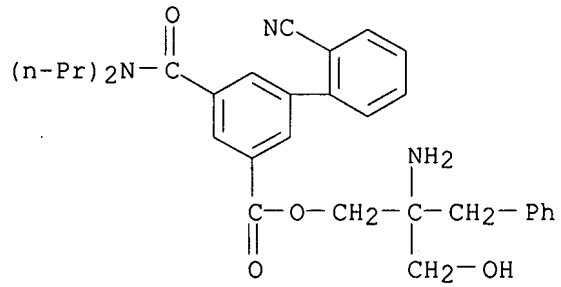
alkenyl, alkynyl, Ph, PhCH2; R7 = H, alkyl, alkenyl, alkynyl; R3 = (substituted) PhCHR5NHCO, R9R10NHCO, etc.; R9R10 = atoms to form (substituted) pyrrolidinyl, piperidinyl; R11 = OH, alkoxy, phenylalkoxy, PhO, Ph; R12 = NR9R10, OH], were prepared as β-secretase inhibitors for the treatment of Alzheimer's disease (no data). Title compound (II) was prepared in several steps.

IT 827039-57-6P 827039-62-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of phenylcarboxylate esters as β-secretase inhibitors for the treatment of Alzheimer's disease)

RN 827039-57-6 CAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid, 5-[(butylmethylamino)carbonyl]-2'-cyano-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)



RN 827039-62-3 CAPLUS
CN [1,1'-Biphenyl]-3-carboxylic acid, 2'-cyano-5-[(dipropylamino)carbonyl]-, 2-amino-2-(hydroxymethyl)-3-phenylpropyl ester (9CI) (CA INDEX NAME)



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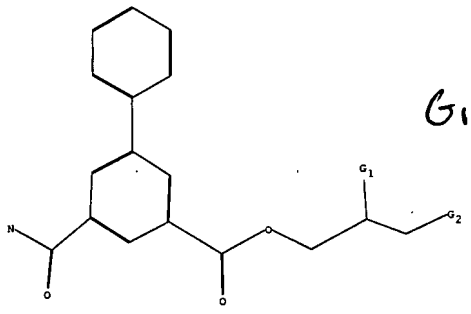

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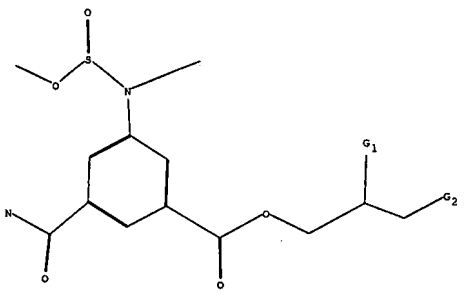

$G_1 = H, O$

$G_2 = O, \text{Phenyl}$